

Loop-Cluster Coupling and Algorithm for Classical Statistical Models

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Potts spin systems play a fundamental role in statistical mechanics and quantum field theory and can be studied within the spin, the Fortuin–Kasteleyn (FK) bond or the q -flow (loop) representation. We introduce a Loop-Cluster (LC) joint model of bond-occupation variables interacting with q -flow variables and formulate an LC algorithm that is found to be in the same dynamical universality as the celebrated Swendsen–Wang algorithm. This leads to a theoretical unification for all the representations, and numerically, one can apply the most efficient algorithm in one representation and measure physical quantities in others. Moreover, by using the LC scheme, we construct a hierarchy of geometric objects that contain as special cases the q -flow clusters and the backbone of FK clusters, the exact values of whose fractal dimensions in two dimensions remain as an open question. Our work not only provides a unified framework and an efficient algorithm for the Potts model but also brings new insights into the rich geometric structures of the FK clusters.

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Introduction.—The understanding of critical phenomena is strongly intertwined with the study of the rich behavior of the q -state Potts model [1]. Aside from the historical spin representation [2,3], two other representations of the Potts model have played a central role: the q -flow representation [4,5], which is a generalization of the loop description, and the Fortuin–Kasteleyn (FK) bond representation [6,7], which is also known as the random-cluster (RC) model. On one hand, theoretical advances were achieved thanks to the geometric and probabilistic interpretations these two representations, as well as the extension to positive real q values [8–10]. For instance, they play an important role in conformal field theory [11] and in stochastic Loewner evolution [12–16]. On the other hand, numerical Monte Carlo methods, decisive in the study of not-exactly-soluble models, have significantly benefited from these insights. Indeed, the Metropolis [17] or heat-bath schemes rely on single-spin moves and often suffer from severe *critical slowing-down* [18,19], and the Sweeny algorithm [20], a local-bond update scheme, has complications from connectivity checking. Based on the coupling between spin and FK representations [6,7,21], efficient cluster methods, including the Swendsen–Wang (SW) and Wolff algorithms [22,23], have been developed and widely used. For the q -flow representation, one can apply the Prokof'ev–Svistunov worm algorithm [24–27], which has proven to be particularly efficient at computing the

magnetic susceptibility [28] and the spin-spin correlation function [29].

However, despite the existence of the coupling between spin and FK representation for decades [6,7,21], a generic coupling between the q -flow and another representation, which would tie the three representations together, has remained an open question.

In this Letter, we propose a unified framework by introducing a joint model, called the Loop-Cluster (LC) model, of FK bond variables interacting with q -flow variables. It includes and provides a straightforward derivation of the coupling for the Ising model [30,31] and applies to the Potts model of any integer $q \geq 1$. The LC joint model provides a setup for a new Monte Carlo algorithm, which we call the Loop-Cluster (LC) algorithm. By investigating the dynamical properties over the complete graph and $d = 2, 3, 4, 5$ toroidal grids, we show that the LC and the SW schemes are in the same universality class. As a consequence, the three representations are tied together, and numerically, one can apply the most efficient algorithm in one representation and measure observables in others, as illustrated in Fig. 1.

Much insight is also gained on the geometric structures of the Potts model from the LC scheme. The q -flow clusters, defined by sets of vertices connected by nonzero flow variables, can be proven to be contained in the backbones of FK clusters. Further, we construct a hierarchy

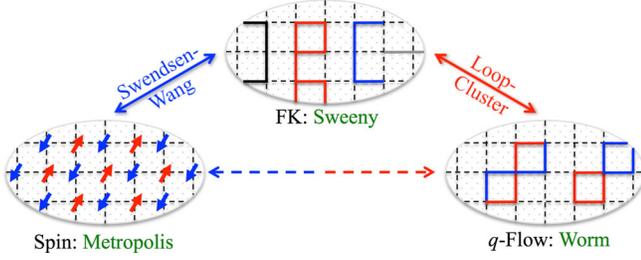


FIG. 1. Representations and algorithms for the Potts model. The spin, q -flow, and FK representations are coupled by the combination of the Swendsen–Wang and the Loop-Cluster algorithm.

of random q_F -flow clusters from a q -state FK configuration with real $q \geq 0$ and integer $q_F \geq 2$, which reduce to the q -flow clusters for $q_F = q$ and the backbones for $q_F \rightarrow \infty$. This provides a new perspective to study the long-standing question about the backbone dimension for percolation and FK clusters [32–38]. In two dimensions (2D), we determine with high precision the fractal dimension d_F for various q_F and q , and conjecture an exact formula for $q_F = 2$. However, for generic (q_F, q) , the exact value of d_F remains unknown, and the exploration might request progresses in conformal field theory.

Representations of the Potts model.—We begin with the introduction of the Potts, q -flow, and RC models. Consider a finite graph $G \equiv (V, E)$, where V is the vertex set and E is the edge set. Let each vertex i be occupied by a Potts spin $\sigma_i \in \{0, 1, \dots, q-1\}$ with $q > 1$ an integer, the q -state Potts model is defined by the probability distribution

$$d\mu_{\text{spin}}(\{\sigma\}) = \mathcal{Z}_{\text{spin}}^{-1} \prod_{(ij)} \exp[J_{ij}(\delta_{\sigma_i, \sigma_j} - 1)] d\mu_0(\{\sigma\}),$$

where $J_{ij} > 0$ is the ferromagnetic coupling for edge $(ij) \in E$ in the graph G , and $d\mu_0(\{\sigma\})$ is the counting measure for the Potts spin configurations. The partition sum $\mathcal{Z}_{\text{spin}}$ acts as a normalization factor. Introducing the edge probability $p_{ij} \equiv 1 - \exp(-J_{ij})$, the Potts distribution can be rewritten as

$$d\mu_{\text{spin}}(\{\sigma\}) = \mathcal{Z}_{\text{spin}}^{-1} \prod_{(ij)} [p_{ij} \delta_{\sigma_i, \sigma_j} + (1 - p_{ij})] d\mu_0(\{\sigma\}). \quad (1)$$

Now, we can assign to each edge $(ij) \in E$ a random bond variable $b_{ij} \in \{0, 1\}$ and define the subgraph $G_b \equiv (V, E_b) \subseteq G$, with E_b consisting of the edges (ij) with occupied bond $b_{ij} = 1$. Let a cluster be a set of vertices connected via occupied bonds, the constraint $\delta_{\sigma_i, \sigma_j}$ requires that all the Potts spins in the same cluster take the same value, while the spin values in different clusters are independent from each other. After summing out the spin degree of freedom, one obtains a FK bond configuration, $\{b\}$, in which each cluster has a statistical weight of q .

The corresponding RC model with parameter q is then defined by the probability distribution

$$d\mu_{\text{FK}}(\{b\}) = \mathcal{Z}_{\text{FK}}^{-1} q^k \prod_{(ij) \in E_b} p_{ij} \prod_{(ij) \notin E_b} (1 - p_{ij}) d\mu_0(\{b\}), \quad (2)$$

where $k \equiv k(G_b)$ is the number of clusters in G_b , including single-vertex clusters.

We can also add to each edge of G a q -flow variable $f_{ij} \in \{0, 1, \dots, q-1\}$ and denote by $G_f \equiv (V, E_f) \subseteq G$ the subgraph of edges (ij) with nonzero flows $f_{ij} > 0$. Further, we introduce the symbol ∂G to represent the set of vertices that do not satisfy the condition given by the q -modular Kirchhoff conservation law as

$$\sum_{j: (ij) \in E} \text{sgn}(i \rightarrow j) f_{ij} = 0 \pmod{q}, \quad \text{for any } i \in V, \quad (3)$$

where $\text{sgn}(i \rightarrow j) = -\text{sgn}(j \rightarrow i) \in \{\pm 1\}$ accounts for the edge orientation. The q -flow model is described by the probability distribution

$$d\mu_{q\text{Flow}}(\{f\}) = \mathcal{Z}_{q\text{Flow}}^{-1} \delta_{\partial G = \emptyset} \times \prod_{(ij) \in E_f} \frac{p_{ij}}{q} \prod_{(ij) \notin E_f} \left(1 - \frac{q-1}{q} p_{ij}\right) d\mu_0(\{f\}), \quad (4)$$

where $\delta_{\partial G = \emptyset}$ means an empty set for ∂G , i.e., no vertex breaks the conservation law. The edge orientations play no physical role and can be randomly chosen, as reversing an edge (ij) orientation can be counterbalanced by mapping the flow variable f_{ij} to $q - f_{ij} \pmod{q}$.

Using high-temperature expansion [4–7, 39], duality relations [1, 40], or low-temperature expansion for 2d-planar graphs, it is known that $\mathcal{Z}_{\text{spin}} = \mathcal{Z}_{\text{FK}} = q^{|V|} \mathcal{Z}_{q\text{Flow}}$ and, thus, apart from an unimportant constant $q^{|V|}$, the Potts, RC and q -flow models are equivalent to each other.

Joint models.—In 1988, Edwards and Sokal defined a joint model [21] having the q -state Potts spin σ_i at the vertices and occupation variable b_{ij} on the edges with probability distribution

$$d\mu_{\text{JSW}}(\{\sigma\}, \{b\}) = \mathcal{Z}_{\text{JSW}}^{-1} \prod_{(ij)} [p_{ij} \delta_{b_{ij}, 1} \delta_{\sigma_i, \sigma_j} + (1 - p_{ij}) \delta_{b_{ij}, 0}] d\mu_0(\{\sigma\}) d\mu_0(\{b\}). \quad (5)$$

On this basis, the SW cluster algorithm can be easily understood as passing back and forth between the spin and FK representations via the joint model, Eq. (5). Given a spin configuration, a random FK configuration is generated as follows: independently for each edge (ij) , one sets $b_{ij} = 0$ for $\sigma_i \neq \sigma_j$ and sets $b_{ij} = 1$ (resp. 0) with probability p_{ij}

[resp. $(1 - p_{ij})$], for $\sigma_i = \sigma_j$. The reverse process starts with a FK bond configuration. One picks equiprobably a σ_i variable from the set $\{0, 1, \dots, q - 1\}$ for each connected cluster and assigns the σ_i value to all the spins in this cluster.

We shall formulate a joint model between the FK bond and the q -flow configurations and the corresponding algorithm that passes back and forth. We first remark that, using the Euler formula $k(G_b) = |V| - |E_b| + c(G_b)$, we can underline the cycle structure in the RC model by rewriting it as

$$d\mu_{\text{FK}}(\{b\}) = \mathcal{Z}_{\text{FK}}^{-1} q^{|V|+c} \prod_{(ij) \in E_b} \frac{p_{ij}}{q} \prod_{(ij) \notin E_b} (1 - p_{ij}) d\mu_0(\{b\}), \quad (6)$$

where $c \equiv c(G_b)$ is the number of independent loops (cycles) in G_b . Further, a simple decomposition in the q -flow model, Eq. (4), leads to

$$d\mu_{q\text{Flow}}(\{f\}) = \mathcal{Z}_{q\text{Flow}}^{-1} \delta_{\partial G = \emptyset} \times \prod_{(ij) \in E_f} \frac{p_{ij}}{q} \prod_{(ij) \notin E_f} \left(\frac{p_{ij}}{q} + 1 - p_{ij} \right) d\mu_0(\{f\}), \quad (7)$$

since zero-valued flows correspond to modulo q either 0 or q (resp. $1 - p_{ij}$ and p_{ij}/q contributions). Analogously to [21], we define a joint model having the bond variable b_{ij} and the flow variable f_{ij} on each edge with the probability distribution

$$d\mu_{\text{jLC}}(\{f\}, \{b\}) = \mathcal{Z}_{\text{jLC}}^{-1} \delta_{\partial G = \emptyset} \prod_{(ij)} \left[\frac{p_{ij}}{q} \delta_{f_{ij} \neq 0} \delta_{b_{ij}, 1} + \frac{p_{ij}}{q} \delta_{f_{ij} = 0} \delta_{b_{ij}, 1} + (1 - p_{ij}) \delta_{f_{ij} = 0} \delta_{b_{ij}, 0} \right] \times d\mu_0(\{f\}) d\mu_0(\{b\}). \quad (8)$$

We call this model the Loop-Cluster (LC) joint model. As the edge state $(f_{ij} \neq 0, b_{ij} = 0)$ is forbidden, i.e., has zero probability, it yields $G_f \subseteq G_b \subseteq G$. By explicitly performing the summation over either the $\{b\}$ or the $\{f\}$ variables, it is easy to verify the following facts about the LC joint model, Eq. (8):

(i) The marginal probability of the flow variables $\{f\}$ is precisely the q -flow model, Eq. (7), since, after summation over the bond states $b_{ij} = 0, 1$, an edge with the flow state $f_{ij} \neq 0$ has the statistical weight p_{ij}/q , and one with $f_{ij} = 0$ a statistical weight of $(1 - p_{ij}) + p_{ij}/q$, as in Eq. (7).

(ii) The marginal probability of the bond variables $\{b\}$ is precisely the RC model, Eq. (6). The summation over the flow variables $\{f\}$ involves the number of choices of

assigning the flow variables under the constraints that $\partial G = \emptyset$ and the state $(f_{ij} \neq 0, b_{ij} = 0)$ is forbidden. This number identifies with the number of possible flow configurations on the subgraph of occupied bonds, i.e., the flow configurations satisfying $\partial G_b = \emptyset$. This number amounts to $q^{c(G_b)}$ by considering the decomposition of the Kirchhoff law, Eq. (3), into the loop flows on the graph G_b . Indeed, once the flow variable of an unshared edge of a loop is determined among the q possible values, it must be propagated along the loop, defining the loop flow. The final flow for a given edge is the sum modulo q of the loop flows in which it is contained. Thus, any bridge edge, i.e., not contained in any loop and whose removal would increase the number of clusters, is assigned a flow zero.

(iii) Given the flow variables $\{f\}$, the bond variables $\{b\}$ are all independent and set by the conditional distribution $p(b_{ij} = 1 | f_{ij} > 0) = 1$ for any edge (i, j) with a nonzero flow, $p(b_{ij} = 1 | f_{ij} = 0) = \{p_{ij} / [p_{ij} + q(1 - p_{ij})]\} \equiv t_{ij}$ and otherwise.

(iv) Given the bond variables $\{b\}$, the subset of flow variables $\{f\}_b$ on a cluster G_b is independent from the others and set by $p(\{f\}_b | G_b) = q^{-c(G_b)} \delta_{\partial G_b = \emptyset}$ and $p(f_{ij} = 0 | b_{ij} = 0) = 1$ for all edges (ij) with unoccupied bonds.

(v) The joint model, Eq. (8), highlights the fundamental relationship between the FK and q -flow representations as both can be understood as the result of a high-temperature expansion over $p_{ij}/(1 - p_{ij})$ and t_{ij} , respectively, revealing either the connected cluster or flow structure. Furthermore t_{ij} identifies with the thermal transmissivity arising in the renormalization group [5,41].

Loop-Cluster algorithm.—We are now ready to formulate an LC Monte Carlo method that simulates the joint model, Eq. (8). To be specific, we alternatively generate new bond variables, independent of the old ones, given the flows following (iii), and new flow variables, independent of the old ones, given the bonds following (iv). The marginal distribution $d\mu_{\text{FK}}$ in Eq. (6) [$d\mu_{q\text{Flow}}$ in Eq. (7)] from the joint model, Eq. (8), is then simply obtained by erasing the flow variables $\{f\}$ (bond variables $\{b\}$), as stated in (i),(ii). This sampling procedure is a generalization of the mapping method proposed in [30,31] for the Ising case.

(A) Given a q -flow configuration, generating a random FK bond configuration is a straightforward local process given in (iii): for each nonzero flow $f_{ij} \neq 0$, one sets $b_{ij} = 1$; for each edge with empty flow $f_{ij} = 0$, one *independently* sets $b_{ij} = 1$ with probability t_{ij} , and $b_{ij} = 0$, otherwise. The number of operations in this step equals the number of edges of the original graph, $|E|$.

(B) Given a FK bond configuration, generating a q -flow configuration follows from (iv) and depends on the subgraph- G_b topology: For all the nonoccupied edges $b_{ij} = 0$, one sets $f_{ij} = 0$; the edges in E_b are assigned flow variables $\{f\}$ as described in (ii), once a set of independent loops have been defined.

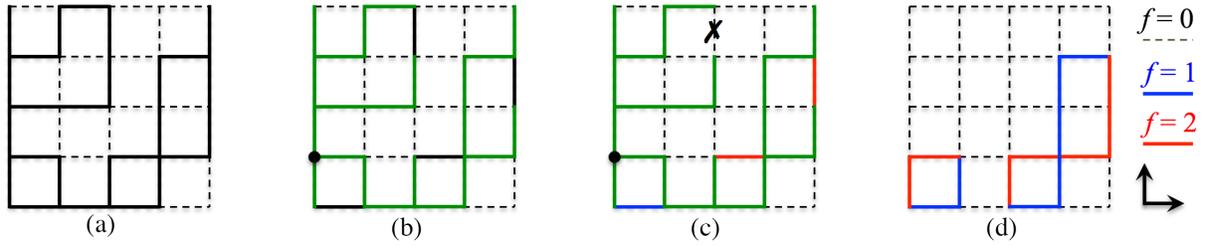


FIG. 2. Illustration of a cluster-to-loop update for $q = 3$, with an up and right orientation, as shown in (d). From an FK bond configuration (a), a spanning tree is constructed from a root vertex, as marked by the green color (b). Each occupied edge missing from the tree defines an independent cycle and is assigned a random flow variable $f \in \{0, 1, \dots, q - 1\}$ (c). Finally, the q -flow variables for all the other edges are obtained by backtracking vertices and applying the q -modular Kirchhoff conservation law for each vertex, yielding a q -flow configuration (d).

In more detail, we first construct a spanning tree for each connected cluster by a rooted procedure, either the breadth-first or the depth-first search. Any occupied edge of the graph G_b missing from the tree defines a loop by the tree paths from the pair of ending vertices of the missing edge to the root vertex. Each of these occupied bonds is uniformly assigned a flow variable $f_{ij} \in \{0, 1, \dots, q - 1\}$. Then, we backtrack the tree and calculate the flow variables for all its edges by applying the q -modular Kirchhoff conservation law to each vertex. The number of operations is twice the number of edges in the original graph, $2|E|$. Figure 2 illustrates an example of “constructing-tree” and “backtracking” processes for $q = 3$. The number of operations is $3|E|$ for the LC scheme, slightly larger than $2|E|$ for the SW algorithm.

For $q = 1$, the set of flow variables $\{0, \dots, q - 1\}$ reduces to $\{0\}$, and the LC algorithm becomes the conventional strategy for bond percolation.

The LC algorithm can be extended to sample from the RC model of real value $q \geq 1$ via the induced-subgraph decomposition [9]. Further, a single-cluster version can be

formulated to sample from the q -flow model. See the Supplemental Material [47] for details.

Dynamical behavior.—We study numerically the dynamics of the LC algorithm and compare it to the SW scheme for both “energylike” and “susceptibilitylike” quantities in the FK representation at criticality over the complete graph and $d = 2, 3, 4, 5$ toroidal grids, where the critical coupling strengths are taken from Refs. [1, 2, 42–45]. By comparing the integrated autocorrelation times, as calculated by a windowing method [46], we obtain clear evidence that both the SW and LC schemes belong to the same dynamical class (even displaying similar decorrelation performance for $q = 2$ in 2D), as well as the Wolff and the single-cluster LC variant. Further details are given in the Supplemental Material [47].

New family of fractal objects.—The FK bond representation provides a platform to study rich geometric structures for any real $q \geq 0$. A variety of fractal dimensions are used to characterize the sizes of FK clusters, the hulls, the external perimeters, the backbones, and the shortest paths, etc., [48,49], and a set of exponents is defined to account for correlation functions that two far-away regions are connected by a number of monochromatic or polychromatic paths [50–52]. In 2D, thanks to Coulomb-gas arguments, conformal field theory, and stochastic Loewner evolution theory, the exact values of most of these exponents are available. For instance, one has the fractal dimension $D_{\text{FK}} = (g + 2)(g + 6)/8g$ for the FK clusters and the correlation exponent $X_2 = 1 - 2/g$ for two polychromatic paths, where the Coulomb-gas coupling $g \in [2, 4]$ relates to q as $q = 2 + 2 \cos(g\pi/2)$ [53–55]. Nevertheless, exact values still remain unknown for a few exponents, including the backbone dimension D_{bb} . For percolation ($q = 1$), while the proximity of the numerical estimates for D_{bb} to the fraction $D_{\text{FK}} - X_2 = 79/48 \approx 1.645833$ has been noticed [32,56], this value seems ruled out by a high-precision study $D_{\text{bb}} = 1.64336(10)$ [37].

As in the FK representation, clusters can be defined as sets of vertices connected via edges of nonzero flows in a q -flow configuration, which have so far received little attention. From the LC joint model, Eq. (8), it is seen that a

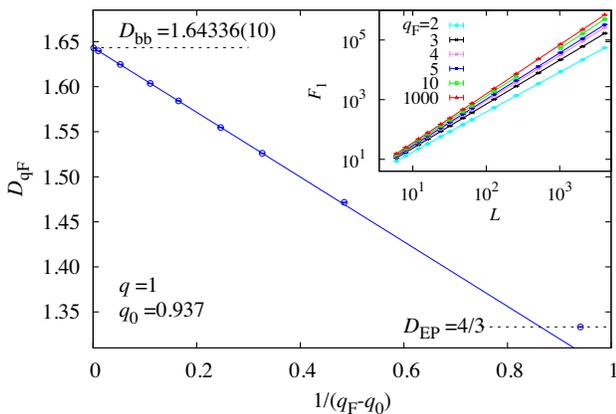


FIG. 3. Convergence of the fractal dimension D_{q_F} of q_F -flow clusters from $D_{\text{EP}} = 4/3$ to the backbone dimension $D_{\text{bb}} = 1.64336$ with $1/(q_F - q_0)$, $q_0 = 0.937$ for the 2D percolation. Inset: scaling of the size F_1 of the largest q_F -flow clusters for increasing value of q_F .

FK cluster may contain more than one q -flow cluster while the reverse cannot occur. Actually, since any bridge edge has a zero flow, the q -flow clusters must live on top of the backbones of the FK cluster sets of vertices connected via nonbridge edges. In practice, since any loop has a flow zero with probability $1/q$, q -flow clusters are generally smaller than the backbone clusters and, therefore, one has $D_{qF} \leq D_{bb} \leq D_{FK}$.

Further, given a q -state FK bond configuration, we can introduce an integer parameter $q_F \geq 2$ such that, in Step B of the LC scheme for assigning flow variables, each loop has a flow zero with probability $1/q_F$ and the q_F -modular conservation law applies to each vertex. This leads to a hierarchy of q_F -flow clusters, reducing to the q -flow clusters for $q_F = q$. Note that Step A can no longer be applied if $q_F \neq q$, and the FK configuration has to be updated by other means like the cluster or Sweeny algorithms [20,22,23].

We carry out extensive simulation for $(q = 1, 2, 3, 2 + \sqrt{3}, q_F = 2)$ and $(q = 1, q_F = 2, 3, 4, 5, 7, 10, 20, 100, 1000)$ on the 2D toroidal grid with linear size $L \in [6, 4096]$. From finite-size scaling analysis, we determine the fractal dimension D_{qF} for the q_F -flow clusters. For $q_F = 2$, the results are $D_{qF} = 1.3333(2) \approx 4/3$, $1.3754(12) \approx 11/8$, $1.417(2) \approx 17/12$, and $1.464(6) \approx 35/24$ for $q = 1, 2, 3, 2 + \sqrt{3}$, respectively. These are well consistent with the external-perimeter fractal dimension $D_{EP} = 1 + g/8$ [54], and, thus, we conjecture $D_{qF}(q_F = 2) = D_{EP}$.

For percolation ($q = 1$), we obtain $D_{qF} = 1.4716(2)$, $1.5261(2)$, $1.5547(2)$, $1.5842(2)$, $1.6036(2)$, $1.6247(2)$, $1.6398(2)$, and $1.6429(2)$ for $q_F = 3, 4, 5, 7, 10, 20, 100, 1000$, respectively. As q_F increases, D_{qF} converges to the backbone dimension asymptotically as $1/(q_F - q_0)$ as shown in Fig. 3. A least-squares fit with $q_F \geq 4$ yields $q_0 = 0.94(4)$ and $D_{qF}(q_F \rightarrow \infty) = 1.6434(2)$, which agrees well with $D_{bb} = 1.64336(10)$ [37].

Conclusion.—We introduce the LC joint model of the FK bond and q -flow representations of the Potts model, unifying its three standard representations. A straightforward application is the design of LC algorithms. While in the same dynamical class as the SW and Wolff methods, the LC algorithms lift the limitation of performing both simulations and measurements in a given representation. More importantly, the LC coupling sheds much new light on the geometric properties of FK and q -flow clusters. It is proved that the q -flow clusters have a fractal dimension not larger than the backbone one of the FK clusters. Further, a hierarchy of q_F -flow clusters is constructed with integer $q_F \geq 2$, enriching the characterization of fractal structures of the FK clusters. In two dimensions, from our high-precision results, we conjecture $D_{qF}(q_F = 2) = D_{EP} = 1 + g/8$; otherwise, the exact values of D_{qF} are not available for generic (q, q_F) . Future works shall focus on an extensive study in the (q, q_F) diagram and seek for the exact formula of D_{qF} in two dimensions.

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