Spin glasses and percolation

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The description of thermodynamic phase transitions in terms of percolation transitions of suitably defined clusters has a long tradition and boasts a number of important successes, the most prominent ones being in ferromagnetic lattice models. Spin glasses and other frustrated systems are not among them as the clusters of aligned spins usually considered in this context start to percolate in the disordered phase and hence fail to indicate the onset of ordering. In this mini-review we provide an overview of the state of the art in this field, including recent advances, and outline the main open questions in the area.

1 Introduction

Percolation models were first proposed and studied by Flory and Stockmeyer in the context of polymer gelation [1, 2], and they have found applications in an astonishingly broad range of areas, from forest fires [3], over porous media in oil fields [4], to electric conductivity [5] and all the way to complex networks [6]. For lattice systems, Broadbent and Hammersley [7] first proposed the idea of what is today known as *bond percolation*, where the edges of a lattice are occupied at random with a probability p, and the resulting structure of connected components is investigated [8]. This model provides one of the simplest and most fundamental examples of a (usually continuous) phase transition. For percolation, the transition is characterized by the appearance of a spanning or *incipient percolating* cluster that connects opposite edges of the system and is of infinite size in the thermodynamic limit. At the transition point, p_c, clusters exist on all length scales and the system is correlated up to the largest distances, forming a (stochastic) self-similar fractal [3].

This behavior is reminiscent of the spatial correlations observed in other systems near criticality, for instance in the magnetic ordering transition of lattice spin models [9]. In view of the success and intuitive appeal of the percolation picture, it has been a longstanding goal in the description of phase transitions and critical phenomena to represent the ordering process in general systems as a percolation transition of suitably defined structures or *droplets* in the substance that form as the phase changes [10]. Fisher proposed a model [11] that postulated droplets of a certain free energy whose average size diverges at the critical point and that feature a cluster size distribution whose exponents are related to the critical indices of the thermal transition. A microscopic definition of such droplets, however, was initially not available. While it was clear that they must correspond to a spatially *correlated* percolation problem, it soon became clear that the clusters (connected components) of like spins do *not* fit Fisher's description as they percolate away from the thermal critical point [12]. Coniglio and Klein [13] first realized that suitable clusters resulted from a merely *probabilistic* occupation of bonds between like spins if the occupation probability was chosen as $p = 1 - \exp(-2\beta J)$, where β is the inverse temperature and J denotes the ferromagnetic exchange coupling. Independently, Fortuin and Kasteleyn [14] had provided a representation of the Potts model in form of a correlated percolation model that contained the same cluster definition. The resulting

Fortuin-Kasteleyn-Coniglio-Klein (FKCK) clusters percolate at the thermal transition point and their structure encodes the nature of spin-spin correlations. They are also the basis for powerful numerical simulation schemes in form of the cluster algorithms of Swendsen and Wang [15] as well as Wolff [16].

While these ideas are rather straightforwardly generalized from Ising to Potts variables, as well as to continuous spins [16], and even to disordered ferromagnets [17], they fail as soon as competing interactions and frustration come into play [18, 19]. Further, while FKCK clusters can be easily generalized to this case by focusing on (parallel or antiparallel) spin pairs with *satisfied* bonds, it is found that in three dimensions such clusters percolate far away from the spin-glass transition point as they, in fact, do *not* encode the relevant correlations at the spin-glass transition [20]. Instead, it has been proposed that one should consider cluster definitions based on overlap variables, as they encode the order parameter of the spin-glass transition [21]. Further, it appears that a more subtle property of clusters than the mere onset of percolation might be associated with the occurrence of the spin-glass transition. Only in two dimensions, where the situation is somewhat different as the spin-glass transition is shifted to zero temperature, does one observe for some types of overlap-based clusters the percolation points asymptotically approach the spin-glass transition [22].

Based on some of these observations, a number of cluster-update algorithms for spin glasses have been proposed, the general target being to ensure that the updated clusters undergo a percolation transition at or close to the spin-glass transition, and that the structure of clusters encodes the correlations of the underlying spin model. A general solution to this problem has not been found to date, but some approaches provide reasonably good performance for systems in two dimensions [23], for spin glasses on diluted lattices [24], or for an intermediate size range in three and higher dimensions [25]. In the remainder of this mini-review, we will provide a more detailed discussion of the connection between percolation and the spin-glass transition and the simulation algorithms based on these observations.

2 Spin clusters

While some of what is discussed below can be generalized to the cases of Potts spins as well as continuous models such as the *XY* and Heisenberg spin glasses, to be specific we focus on the case of the short-range (Edwards-Anderson) Ising spin glass with Hamiltonian [26]

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j, \tag{1}$$

where $\sigma_i = \pm 1$ and the sum is taken over nearest-neighbor pairs of the lattice only. To allow for a spin-glass phase, the distribution of the quenched couplings J_{ij} should include values of both signs, the most common cases being the bimodal and Gaussian distributions. In a natural generalization from the cases of ferromagnetic Ising and Potts models, FKCK clusters may be constructed for such a system by occupying bonds between *satisfied* spin pairs, i.e., those with $J_{ij}\sigma_i\sigma_j > 0$, with probability

$$p_{\text{FKCK}} = 1 - \exp\left[-2\beta|J_{ij}|\right]. \tag{2}$$

There is clear numerical evidence that such clusters percolate at temperatures far above the spin-glass transition, for instance at $T_{\text{c,FKCK}} = 3.934\,(3)$ for the three-dimensional symmetric $\pm J$ model [19, 20] as compared to the spin-glass transition temperature at $T_{\text{SG}} = 1.101\,(5)$ [27] (a similar difference is expected for the model with Gaussian couplings). In two dimensions, these clusters percolate at $T_{\text{SG}} = 1.1894\,(3)$ for the Gaussian model [22], while the spin-glass transition only occurs for $T \to 0$ [28]. More generally, for a bimodal model with a fraction x of antiferromagnetic bonds with $J_{ij} < 0$, a coincidence of the percolation transition and the thermal transition point is only observed for $x = 0$ [20]. This behavior is rather plausible since FKCK clusters do not represent the relevant spin correlations in these systems. While for the ferromagnet [29]

$$\langle s_i s_j \rangle = \text{Prob}\,(i \text{ and } j \text{ are connected by occupied bonds}), \tag{3}$$

the situation for spin glasses is more subtle, and one can show that in this case [21, 30]

$$
\begin{aligned}
\langle s_i s_j \rangle = \ &\text{Prob}\,(i \text{ and } j \text{ are connected by an even number} \\
&\quad \text{of occupied antiferromagnetic bonds}) \\
&- \text{Prob}\,(i \text{ and } j \text{ are connected by an odd number} \\
&\quad \text{of occupied antiferromagnetic bonds}).
\end{aligned}
\tag{4}
$$

Hence, the percolation of FKCK clusters no longer implies the presence of long-range order. Since the percolation transition of FKCK clusters does not encode spin-glass criticality (but see Ref. [31] for a possible connection to damage spreading), it is expected that it is in the universality class of random percolation, and this expectation is borne out by the results of numerical simulation studies [20, 22, 32] as well as rigorous analysis [33, 34].
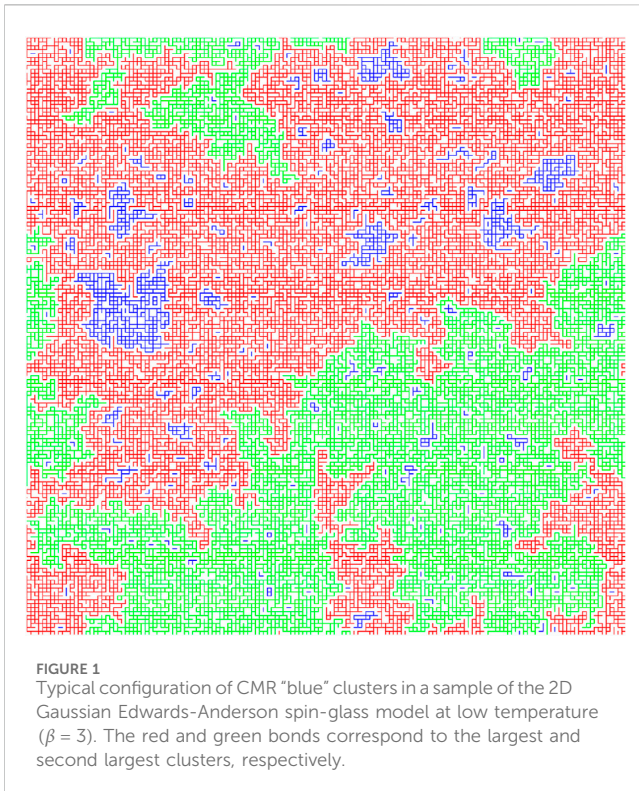
3 Overlap clusters

This failure is not surprising in view of the fact that the magnetization is no order parameter for the spin-glass transition and, instead, for its description one needs to turn to *overlap* variables [35]. Several cluster definitions have been suggested based on the site or link overlap of two spin configurations using the same disorder realization. Initially in the context of random-field models, Chayes, Machta and Redner [36] proposed a representation where doubly satisfied ("blue") bonds in a two-replica representation are occupied with a probability

$$p_{\text{CMR,blue}} = 1 - \exp\left[-4\beta|J_{ij}|\right], \tag{5}$$

while, additionally, singly satisfied ("red") bonds are occupied with probability

$$p_{\text{CMR,red}} = 1 - \exp\left[-2\beta|J_{ij}|\right].$$

Then, it is possible to relate the percolation properties of such clusters to the occurrence of symmetry breaking of the spin system [21]: in contrast to the ferromagnet, where the appearance of a percolating cluster suffices to indicate the onset of the ordered phase, for spin glass there should be a "blue" cluster of strictly larger density than any other cluster [37]. In practise, one observes the occurrence

FIGURE 1
Typical configuration of CMR "blue" clusters in a sample of the 2D Gaussian Edwards-Anderson spin-glass model at low temperature ($\beta = 3$). The red and green bonds correspond to the largest and second largest clusters, respectively.

of *two* percolating clusters of opposite overlap that develop a density difference at the spin-glass transition [21, 22]. A corresponding overlap configuration is shown in Figure 1 for the example of the 2D Gaussian spin glass, illustrating that there are mainly two large clusters of opposite overlap, with any further clusters being much smaller. If the weight of such smaller clusters diminishes for systems of increasing sizes, the overlap q (i.e., the order parameter) is connected to the density difference of the two largest clusters. This is rigorously the case in the mean-field Sherrington-Kirkpatrick model [21], and numerical data in 3D [21] and 2D [22] are also consistent with such a picture—for the 2D case this is demonstrated by the data shown in Figure 2 that consist of the densities of the three largest clusters as a function of inverse temperature and for different lattice sizes. The onset of percolation of CMR blue clusters itself again occurs away from the spin-glass transition, with $T_{c,CMR} \approx 3.85$ for the 3D bimodal model [21] (which is surprisingly close to $T_{c,FKCK}$); in 2D the CMR percolation temperatures of finite lattices converge to $T = 0$ for $L \rightarrow \infty$ [22], consistent with the spin-glass transition temperature there.

Another possible cluster definition based on the overlap of two replicas results from a simple duplication of the FKCK construction on the two spin configurations, i.e., bonds are occupied independently in the two replicas according to the FKCK probability (Eq. 2), and clusters are constructed over all bonds simultaneously occupied in *both* replicas [38]. This is equivalent to a bond occupation probability

$$p_{TRFK} = \left(1 - \exp\left[-2\beta|J_{ij}|\right]\right)^2 \qquad (6)$$

for doubly satisfied bonds. Such clusters might be referred to as two-replica Fortuin-Kasteleyn (TRFK) clusters. These clusters behave

rather similarly to the CMR ones [21, 22], which is not surprising as they follow the same construction apart from the smaller bond occupation probability $p_{TRFK} \leq p_{CMR,blue}$. The latter leads to a significant suppression of the percolation point which now occurs for $T_{c,TRFK} \approx 1.77$ [21].

Finally, a cluster definition based on a *site* percolation problem rather that a *bond* percolation one was first proposed in connection with a specific cluster-update algorithm for spin glasses in 2D [23]. There, clusters are grown in regions of constant overlap, and neighboring sites of the same overlap are *unconditionally* added to the cluster, such that the effective bond occupation probability is
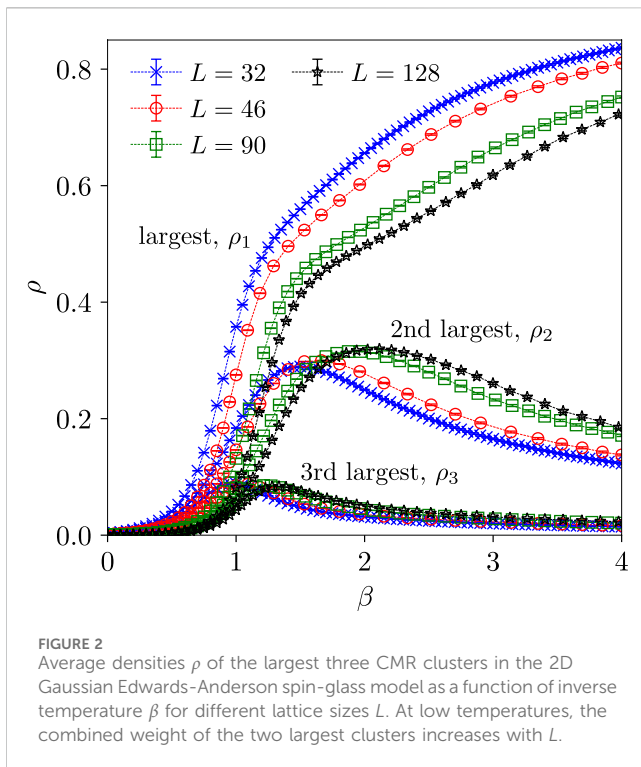
$$p_{Houdayer} = 1.$$

One might hence think of these as some form of *geometric clusters* in overlap space [39]. The CMR and TRFK clusters clearly are subregions of the Houdayer clusters as for the latter one does not take into account whether a given bond is satisfied or not. In many 3D lattices such as the simple cubic one, such clusters percolate already for $T_{c,Houdayer} = \infty$ as their site percolation thresholds are $p_c < 0.5$. Hence they have not been studied in much detail there. In 2D, on the other hand, they again percolate at a sequence of temperatures that approaches $T_{SG} = 0$, but they are found to be in general larger that the CMR and TRFK clusters [22].

4 Cluster updates

In view of the spectacular success of cluster updates in alleviating critical slowing down for ferromagnetic spin models [15, 16] it has been a natural idea to use cluster moves to counter the dramatically slow dynamics observed in spin-glass systems. In fact, the first proposal in this direction [40] even (slightly) predates the ferromagnetic algorithms. Unfortunately, the cluster component in this approach was not found to be extremely efficient, while the replica component eventually lead to the development of the replica exchange or parallel tempering method [41, 42] that is the *de facto* standard for spin-glass simulations.

Houdayer's proposal [23] for a cluster update for 2D models was in this sense more successful. Geometric clusters are constructed in the way described above, by connecting neighboring sites of equal overlap, and an update consists of flipping the spins inside a cluster in *both* replicas. Crucially, such updates can be performed unconditionally, i.e., without adding an extra acceptance step, since they leave the total energy of the replicated system invariant. Usage of more than two replicas (per temperature) is possible, but usually not found to be efficient computationally [43]. Due to the fixed energy, it is clear that such updates are not ergodic, and hence need to be complemented, e.g., by single-spin flip moves. While this approach works well on the square lattice, where the percolation threshold $p_c \approx 0.59 > \frac{1}{2}$ and the percolation points of Houdayer clusters approach $T_{SG} = 0$ for $L \rightarrow \infty$ [22], the method is not very efficient in 3D, which is blamed on the fact that, for most lattices in 3D, $p_c < \frac{1}{2}$ [23]. In an attempt to improve on this aspect, Zhu et al. [25] proposed a modification of Houdayer's method where

FIGURE 2
Average densities ρ of the largest three CMR clusters in the 2D Gaussian Edwards-Anderson spin-glass model as a function of inverse temperature β for different lattice sizes L. At low temperatures, the combined weight of the two largest clusters increases with L.

they grow a single cluster in the *minority* phase of the overlap, which is claimed to somewhat improve the performance in 3D. More recently, the cluster selection for updates has been scrutinized in a multi-cluster version of the algorithm discussed in the context of combinatorial optimization problems [44], a close relative of spin-glass problems (see, e.g., Ref. [45]).

The CMR representation also suggests several cluster updates. Constructing only the blue clusters, these can flip freely as the cluster construction rules together with the bond occupation probability (Eq. 5) mean that the update satisfies detailed balance with respect to the equilibrium distribution [22]. This was used by Jörg [24] to efficiently simulate spin glasses on diluted lattices, leading to overall smaller clusters. By construction, however, the update is not ergodic since spins connected by (partially) unsatisfied bonds cannot be updated. An extension proposed in Ref. [36] (see also [21]) uses both red and blue bonds to construct blue and *grey* clusters, leading to a rejection-free and ergodic update which, however, is still found to be relatively inefficient due to the onset of cluster percolation above T_{SG} [21].

5 Discussion

While a percolation perspective onto spin glasses and other frustrated systems has not led to the same level of revolutionary success this approach has seen for ferromagnets, significant progress has been possible. The cluster construction rules used for ferromagnets (Fortuin-Kasteleyn–Coniglio-Klein), while applicable to spin glasses, do not lead to structures that reflect spin-glass correlations. Instead, clusters must be constructed in overlap space, corresponding to the order parameter of the spin-glass transition. While there is no one-to-one correspondence between the spin-glass transition and a simple percolation transition of a cluster type that has been investigated to date, an intriguing picture has emerged: for the CMR and TRFK clusters defined on two replicas *two* equally large percolating clusters appear significantly above the spin-glass transition, and it is only at the spin-glass transition that their densities start to differ [21, 22]. It appears that below the percolation point smaller clusters beneath the two dominating ones are asymptotically irrelevant.

Regarding cluster updates, a fundamentally efficient algorithm only exists in two dimensions, while attempts for more general, and in particular, 3D systems have only partially been successful. While some improved results where found in cases where the average sizes of clusters constructed are reduced such as in diluted systems [24] or with algorithmic modifications [25], it is not fully clear whether such size reduction is a sufficient condition for improving performance.

In view of this state of affairs a number of interesting questions remain to be addressed in future studies. Is it possible to construct clusters that percolate at or very close to the temperature of the spin-glass transition? One promising direction in this respect is the study of *multi-replica* overlaps [22]. In view of Eq. 6 it is clear that, depending on their precise construction, such clusters could percolate at lower and lower temperatures as the number of replicas is increased. Regarding the algorithms, it was seen that for blue clusters there are two very dominant large clusters in the vicinity of the glass transition, such that in contrast to the ferromagnetic case close to the transition there is no multi-scale nature of spin updates for such blue clusters close to the spin-glass transition. This is likely the prime reason for the unsatisfactory performance of such algorithms. In contrast, for Houdayer's algorithm and its extensions, what is the cluster-size distribution? How do multi-cluster variants of such algorithms perform as compared to the default single-cluster ones? Answers to (some of) these questions hold the potential for significantly advancing our understanding of the spin-glass transition while simultaneously facilitating much improved efficiency in simulating spin-glass systems with the hope of answering some more of the fundamental open questions of this field.

Author contributions

Conflict of interest

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