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# Clusters in frustrated systems

# Antonio Coniglio

Dipartimento di Scienze Fisiche, Università di Napoli, INFM Unità di Napoli, Monte S. Angelo, 80126 Napoli, Italy

#### Abstract

Clusters in frustrated systems are studied in the context of the frustrated percolation model. This model, which contains frustration and connectivity as an essential ingredient, exhibits a large degree of complexity in both static and dynamics. The bond version of the model maps on the spin glass model, while the site version can be applied to a large variety of frustrated systems such as glasses and granular materials. © 2002 Elsevier Science B.V. All rights reserved.

#### 1. Introduction

Clusters concepts have been extremely useful in critical phenomena to elucidate the mechanism underlying a thermodynamic transition [1–3]. Here we want to review some ideas which have been developed in the past few years to explore the possibility of using cluster concepts in frustrated systems. This approach has lead to the development of a generic model, which may be applied to a large variety of systems where frustration plays a dominant role. In particular, the model can be implemented to gain insight into the phenomenology of complex systems such as spin glasses, glasses and granular materials.

In the ferromagnetic Ising model, the thermodynamical transition can be described in terms of clusters made of parallel spins connected by "fictitious" bonds [4]. Using this cluster formalism, the Ising model can be mapped exactly on to a bond percolation model [5,6], consequently the correlation length and the connectedness length (the cluster size linear dimension) coincide and diverge at the Ising critical point. Based on the properties of these clusters, Swendsen and Wang [7] have implemented a fast cluster dynamics, which drastically reduces the critical slowing down.

E-mail address: coniglio@napoli.infn.it (A. Coniglio).

The same formalism generalized to frustrated spins systems maps exactly the spin glass (SG) model onto a new bond percolation model [8,9], which contains geometrical frustration as essential ingredient. This model, which has been called frustrated percolation (FP), exhibits properties which are drastically different from the corresponding unfrustrated case.

As random percolation has been useful to describe a large variety of problems in which connectivity plays a major role [10], in the same way the FP model may be able to describe complex systems where frustration and connectivity are the main ingredients.

## 2. Clusters in the Ising model

Let us briefly recall the cluster formalism for the Ising model. Consider the Ising hamiltonian with nearest neighbour interaction.

$$-H = J \sum_{\langle ij \rangle} (S_i S_j - 1), \qquad (1)$$

where  $S_i = \pm 1$  and the sum is over the nearest neighbour pairs of spins.

Suitable clusters can be defined [4] by putting bonds at random between parallel spins with a probability  $p = 1 - \exp(-2J/k_BT)$ . A cluster is defined as the maximal set of spins connected by bonds. It can be shown [11] that the weight for a bond configuration C to occur, independent on the spin configuration, is given by

$$W(C) = p^{|C|} (1 - p)^{|A|} q^{N(C)}.$$
(2)

Here q=2, |C| is the number of present bonds, |A| the number of edges of the lattice without bonds N(C) is the number of clusters. It can also be shown that the partition function of the Ising model can be expressed in the following Fortuin and Kasteleyn cluster formalism as

$$Z = \sum_{C} W(C) \tag{3}$$

while the pair correlation function  $g_{ij} \equiv \langle S_i S_j \rangle$  coincides with the pair connectedness function  $p_{ij}$ 

$$g_{ij} = p_{ij} , (4)$$

where  $p_{ij}$  is the probability that sites i and j are connected by at least one path of bonds. Consequently, correlation length and connectedness length coincide and clusters made of parallel spins connected by bonds percolate at the Ising critical point, with Ising exponents.

For general q, (3) reproduces the partition function of the q-state Potts model in the cluster formulation. In particular, taking the limit q=1 one recovers the weight of the random bond percolation problem.

#### 3. Clusters in the Ising spin glass model

Consider now the  $nn \pm J$  Ising SG model [12]:

$$-H = J \sum_{\langle ij \rangle} (\varepsilon_{ij} S_i S_j - 1), \qquad (5)$$

where the nearest neighbour interactions  $J_{ij} = J\varepsilon_{ij} = \pm J$  are randomly distributed. A concept crucial in spin glasses is frustration. A loop is frustrated when the spins cannot satisfy all pairs of interactions along the loop. It is easy to verify that a loop is frustrated if and only if the product of the signs of the interactions  $\varepsilon_{ij}$  along the loop equals -1. For a given set of interactions  $\{J_{ij}\}$ , the partition function is given by

$$Z\{J_{ij}\} = \sum_{\{S_i\}} e^{-\beta H} . {6}$$

For low temperature, the SG phase is characterized by the Edwards-Anderson order parameter which is different from zero in the SG phase and goes to zero at the SG temperature  $T_{sq}$ . Above  $T_{sq}$ , one can also define the spin-spin pair correlation function

$$g_{ij} \equiv \langle S_i S_i \rangle \,, \tag{7}$$

where  $\langle \cdots \rangle$  stand for the thermal average for a fixed configuration of interactions  $J_{ij}$ . The length  $\xi$  associated with  $\overline{g_{ij}^2}$  (where the bar stands for the average over all the interaction configuration) diverges as the SG temperature  $T_{sg}$  is approached.

Dynamically, one finds that also the relaxation time diverges at  $T_{sg}$ . However, there are precursor phenomena already at a temperature much larger than the SG temperature. In fact a typical autocorrelation function f(t) decays for large t in a non-exponential form well fitted by a Kohlrausch-Williams-Watts function also known as "stretched exponential", below some temperature  $T^*$  and as a simple exponential above  $T^*$ . In 3D  $T^* \sim 4$  while  $T_{sg} \sim 1.1$ . The numerical results of Ogielski [13] is consistent with  $T^* = T_c$  where  $T_c$  is the critical temperature of the ferromagnetic Ising model. This result supports the argument of Randeira et al. [14] who suggest the onset  $T^*$  of the non-exponential behaviour should be greater than or equal to the Griffiths temperature  $T_c$ . This behaviour is caused by the existence of compact ferromagnetic-type clusters of interactions, the same that are responsible of the Griffiths singularity [15].

The presence of non-exponential relaxation in this approach is therefore a direct consequence of the quenched disorder. Therefore, Randeira's argument does not apply to fully frustrated spin models, where due to absence of disorder there is no Griffiths phase. Nevertheless, numerical results [16] have shown the presence of stretched exponential behaviour in both 2 and 3 dimensions below a temperature T\* much larger than the thermodynamical critical temperature of the fully frustrated model.

We will see that the cluster approach to both frustrated spin systems and spin glasses predicts a percolation temperature where precursor phenomena are expected to occur even when the Griffiths phase is absent.

Now I want to illustrate how the cluster approach for the ferromagnetic Ising model can be extended to frustrated spin systems and as a particular case to the Ising SG model [8]. To fix the ideas, let us consider the spin model (5) for a fixed realization of

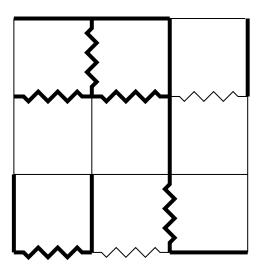


Fig. 1. Bond configurations in the FP problem. Straight and wavy lines indicate positive and negative interactions, respectively. Present bonds are denoted by heavy lines. Configurations of bonds which contain a frustrated loop are not allowed.

interactions  $\{J_{ij}\}$ . As for the ferromagnetic Ising model, we define clusters by randomly putting bonds only between those spins that satisfy the interaction, i.e., we put bonds with probability  $p = 1 - e^{-2\beta J}$ , between only those spins for which  $\varepsilon_{ij}S_iS_j = 1$  and a cluster is defined as the maximal set of spins connected by bonds.

An inspection at the bond configurations shows a major difference compared with the ferromagnetic case. In fact, since bonds can only be between spins satisfying the interaction, we can never have bond configurations which contains frustrated loops. For each configuration of interactions  $\{J_{ij}\}$ , it can be shown that the weight W(C) for a bond configuration C to occur, independent on the spin configuration, is given by

$$W(C) = p^{|C|} (1 - p)^{|A|} q^{N(C)}$$
(8)

if the configuration of bonds C does not contain any frustrated loop, and

$$W(C) = 0$$
 otherwise. (9)

Here q=2, |C| is the number of present bonds, |A| is the number of edges of the lattice without bonds and N(C) is the number of clusters (see Fig. 1). Eq. (9) stems from the fact that a bond configuration which contain a frustrated loop can never occur.

It can also be shown that the partition function (6) can be written as

$$Z\{J_{ij}\} = \sum_{C} W(C). \tag{10}$$

Sometimes, it is convenient to express the weight (9) in terms of the bond chemical potential  $\mu_b$ 

$$W(C) = Ae^{\beta\mu_b|C|}q^{N(C)}, \qquad (11)$$

where  $e^{\beta \mu_b} = p/(1-p)$  and  $A = (1-p)^{\mathcal{N}}$ ,  $\mathcal{N}$  being the number of the total edges in the lattice.

By taking the average of  $\ln Z\{J_{ij}\}$  over all the realizations of interactions, we obtain the free energy of the Ising SG model. In this cluster formulation, the partition function (10) is the analogue of (3) in the ferromagnetic Ising model, except that in the SG case, due to (9), the sum in (10) runs only over those bond configurations which do not contain frustration.

We note that in this formulation the spin variables have disappeared, and the SG model is mapped onto a geometrical problem. In particular, the ground state at T=0 is obtained by packing the maximum number of bonds under the constraint that the bond configurations do not contain a frustrated loop.

Like in the ferromagnetic Ising model, it is possible to express thermal quantities in terms of connectivity functions. For example, it can be shown [8] that the pair correlation function  $g_{ij} \equiv \langle S_i S_j \rangle$  is given by

$$g_{ij} = p_{ij}^+ - p_{ij}^- \,, \tag{12}$$

where  $p_{ij}^+$  ( $p_{ij}^-$ ) is the probability that (1) sites i and j are connected by at least one path of bonds, and (2) the product  $\eta_{ij}$  over all the signs  $\varepsilon_{mn}$  along the path connecting i and j is +1 (-1). Due to the property that the pair correlation function in (12) is given by the difference of two pair connectedness functions,  $|g_{ij}|$  is smaller then the total pair connectedness function  $p_{ij}$ , which for each interaction configuration is given by

$$p_{ij} = p_{ii}^+ + p_{ii}^- \,. \tag{13}$$

Therefore, in SG there are two lengths: one length  $\xi$  associated with  $\overline{g_{ij}^2}$  which diverges at the SG transition temperature  $T_{sg}$  and a second length  $\xi_p$  associated with  $\overline{p_{ij}}$  which diverges at the percolation temperature  $T_p > T_{sg}$  (in 3D  $T_p \sim 3.95$  [17]).

In view of the geometrical interpretation of  $g_{ij}$ , we can understand the SG transition from a different point of view. This transition, like the quantum percolation transition [18], occurs at a temperature lower than the usual percolation transition, due to the interference of paths with different phases. However, at high bond density (low temperature), the interference effects tend to vanish. In fact the number of allowed configurations is extremely reduced and most of the configurations in which i and j are connected will have a common path and, therefore, the same phase. We call this path a "quasifrozen" path since in a dynamical sequence of configurations exploring the allowed phase space, this path will be present most of the time [9,19].

Therefore,  $|g_{ij}|$  roughly coincides with the probability that i and j belong to the same quasifrozen cluster, and the length  $\xi$  associated with  $\overline{g_{ij}^2}$  roughly represents the linear dimension of these clusters. Since  $\xi$  diverges at  $T_{sg}$ , we can interpret the SG transition as a percolation transition of the quasifrozen clusters.

<sup>&</sup>lt;sup>1</sup> It is possible to show that  $p_{ij}^+(p_{ij}^-)$  coincide also with the probability that i and j are connected and the spins at i and j are parallel (antiparallel) in the configurations of spins and bonds.

Indeed, numerical simulations on quasi frozen clusters of nearest neighbour of pairs of spins are consistent with this picture [20,21]. For further interesting developments see Ref. [22].

# 4. Bond frustrated percolation

In the previous section, we have introduced the cluster formulation of the partition function of an Ising SG, which is given by (10) with q = 2. As for the ferromagnetic case, this partition function can be generalized to any q. The percolation model associated to the bond configurations with weights given by (8), (9) is called bond FP. For any q the model can be obtained from a hamiltonian formalism [23,9].

Although the model can be derived from a hamiltonian formalism, it may be convenient to define the FP model more directly as a geometrical problem in the following way:

- (1) Given a lattice assign at random, a configuration of interaction  $\{J_{ij}\}$  on a lattice.
- (2) Assign to any configuration C of bonds a weight W(C) given by (5).

For each configuration of interactions  $\{J_{ij}\}$ , one has to calculate the partition function and any other quantity using the weight given by (8), (9) and then average over all interaction configurations.

The static properties of the FP model have been investigated by using the hamiltonian formalism and solving [24] the model for any q on the hierarchical lattice, introduced by Mckay et al. [25]. The results corroborated also by computer simulations in 2- and 3-dimensions [26,27] and mean field theory [28] show the existence of two critical points.

- (1) A percolation transition at  $T_p(q)$  with critical exponents of the ferromagnetic q/2-state Potts model.
- (2) A glass transition at  $T_0(q)$  in the same universality class of the SG model.

Each critical point is characterized by a diverging length, associated, respectively, with the quantities (12) and (13).

The length  $\xi_p$  associated with the pair connectedness function diverges at the percolation temperature  $T_p$ . The second length  $\xi$  associated with  $\overline{g_{ij}^2}$  diverges at the lower transition temperature  $T_0$ .

The free energy exhibits a singularity not only at  $T_0(q)$  but also at the percolation transition, except in the SG case (q=2), where the amplitude of the singularity vanishes at  $T_p(2)$ . The critical part of the free energy  $F_c$  is thus expected to behave near the percolation threshold  $T_p(q)$  in the following way:

$$F_c = A(q)(T - T_p(q))^{2-\alpha(q)}, (14)$$

where A(q) is an amplitude which vanishes as  $q \to 2$  and  $\alpha(q)$  is the specific heat exponent of the q/2 ferromagnetic state Potts model.

The FP model can also be extended to the case in which the interactions are fixed and not random like in the fully frustrated model, where each plaquette is frustrated. In this case the second transition is in the same universality class of the spin model

with the same distribution of interactions, while the first percolation transition is still in the universality class of ferromagnetic q/2-state Potts model.

If the interactions do not contain any frustration, the two transitions coincide resulting in the standard cluster formalism of the ferromagnetic Potts model [4,5,7]. In this case the amplitude A(q) vanishes in the limit  $\rightarrow 1$ .

Using the cluster formalism, a dynamics can be introduced by removing or adding a bond in such a way to satisfy detailed balance. This generalizes the algorithm, introduced by Sweeny for the cluster formalism of the ferromagnetic q state Potts model. With such algorithm, the FP model can be studied numerically for any value of q including q=1 [26]. Using such dynamics, we have calculated [26] the autocorrelation functions for q=2 and found that the onset of stretched exponential is numerically consistent with  $T_p$  for both fully frustrated and random interactions (spin glasses). Similar results hold also for q=1.

On the other hand for q=2, we can consider the original spin model (5) and apply the spin flip dynamics. It is found numerically that the onset of stretched exponentials once again coincides with  $T_p$  for the fully frustrated hamiltonian, and with the Griffith temperature  $T_c$  which is higher than  $T_p$  for the SG model [16,27]. These findings show that both the percolation transition and the Griffith temperature induces a dynamical anomalies in the form of effective stretched exponentials. In the fully frustrated model, which exhibits only a percolation transition and not the Griffiths singularity, the onset of stretched exponentials occurs, in fact, at the percolation temperature. However in the SG model, which exhibits both the percolation transition and the Griffiths singularity, the onset of stretched exponentials appear at the highest of the two temperatures, namely  $T_c$ .

#### 5. Site frustrated percolation

We consider now the site version of the FP model. We start with the following SG model diluted with lattice gas variables:

$$H = -J \sum_{\langle ij \rangle} (\varepsilon_{ij} S_i S_j - 1) n_i n_j - \mu \sum_i n_i . \tag{15}$$

Here the occupancy variables  $n_i = 0, 1$  have an internal degree of freedom.  $S_i \pm 1$ ,  $\varepsilon_{ij} = \pm 1$  are quenched random interactions and  $\mu$  is the chemical potential for the particles.

This model reproduces the  $\pm J$  Ising SG in the limit  $\mu \to \infty$ , all sites are occupied  $(n_i=1)$ . In the other limit  $J\to\infty$  the model describes a frustrated lattice gas. In fact the first term of Hamiltonian (15) implies that two nearest neighbour sites can be occupied only if their spin variables satisfy the interaction i.e., if  $\varepsilon_{ij}S_iS_j=1$ , otherwise they feel an infinite repulsion  $(J=\infty)$ . Therefore, the particles must either move apart or change the relative orientation of the spins. Since in a frustrated loop the spins cannot satisfy all the interactions, in this model particle configurations in which a frustrated loop is fully occupied are not allowed.

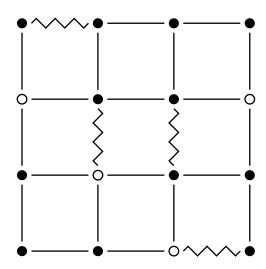


Fig. 2. A configuration of particles (filled circles) and holes (empty circles) in the site FP model.

In the limit  $J \to \infty$ , the partition function of model Hamiltonian (15), after summing over the spin variables, can be written in the cluster formalism as

$$Z = \sum_{C} e^{\beta \mu n(C)} q^{N(C)}, \qquad (16)$$

where q=2 and the sum is over all particles configurations C which do not contain a frustrated loop, n(C) is the number of particles and N(C) is the number of clusters of nearest neighbours particles in the configuration C (Fig. 2). The partition function (16) can be generalized to any value of q [9,29] and gives the site version of the corresponding cluster bond formulation ((10) and (11)).

The connectivity quantities can be related to the thermal ones in the same way as in the bond case (12), (13) and the corresponding percolation model is called site FP. Using the cluster formalism, the site FP model can be studied numerically using the corresponding dynamics of the bond frustrated model. Particles move under the constraint that frustrated loops are not allowed. The strong effect of frustration on particle motion can be seen by allowing the particles to diffuse such that no frustrated loops become completely occupied [29]. At low particle densities, motion is not inhibited by frustration because of the abundance of holes. However, at high densities, a given particle can diffuse through the system only by a large scale, cooperative rearrangement of many particles. At high density, the properties of the site FP for q=1 are not much different from higher values of q. Since the case q=2 can be realised also by the frustrated lattice gas model, namely by using Hamiltonian (15) in the limit of  $J=\infty$ , it is simpler to study the case q=2 using standard techniques applied to the model Hamiltonian (15).

## 6. Frustrated lattice gas

The static properties of the model (15) have been studied in mean field theory [31,32,34]. Interestingly enough, the model in the limit of large J exhibits static properties closely related to the so-called p-spin model [33], which has received much attention since the mean field version of this model gives a good description of glassy behaviour of supercooled liquids.

In finite dimensions, numerical simulation have shown glassy behaviour at high density [30,34,35]. More precisely recent large scale simulations in 3D have shown [37] at high density a SG-like transition in the spin variables, signaled by the divergence of the non-linear susceptibility, and the presence of a continuous replica symmetry breaking in the spin overlap distribution. Moreover, as the critical point is approached from low density, the relaxation time associated with the equilibrium autocorrelation function diverges. On the other hand, the density variables seem to be affected little by the spin variable transition, showing no divergence either in the non-linear compressibility, or in the autocorrelation time.

The freezing of the model is therefore connected with a second-order transition in the spin variables, more similar to the freezing of the Ising SG than to the mode-coupling transition of structural glasses. One cannot exclude, however, that the density variables undergo a glass transition of *p*-spin-like nature at a higher density, characterized by a 1-step replica symmetry breaking and a discontinuity of the Edwards–Anderson parameter defined in terms of density variables. This fact is suggested by the development of a secondary peak in the density overlap distribution at very high chemical potential, as well as by the measurements of the off-equilibrium fluctuation–dissipation ratio [39], but more work is needed to clarify this point.

#### 7. Frustrated lattice gas with annealed disorder

The frustrated lattice gas model contains quenched interactions, while in supercooled liquids the disorder, is not quenched. In order to study the effect of quenched disorder compared to annealed disorder, a variant of the model has been considered in which the interactions evolve in time with a suitable kinetic constraint [36]. Namely, the sign of the interactions  $\varepsilon_{ij}$  are allowed to change only if the sites i and j and all their nearest neighbours are empty. Now the model does not exhibit any thermodynamic transition, however, it shows a dynamical behaviour closely related to some results on the p-spin model in mean field and Lennard–Jones mixture recently found by Franz et al. [38]. Here we show the results for the relaxation of the self-overlap, which is defined as

$$q(t) = \frac{1}{N} \sum_{i} S_i(t') n_i(t') S_i(t'+t) n_i(t'+t)$$
(17)

and for the dynamical susceptibility

$$\chi(t) = N[\langle q(t)^2 \rangle - \langle q(t) \rangle e^2], \qquad (18)$$

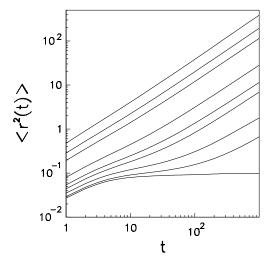


Fig. 3. Self overlap as a function of time in the annealed model, for a system of size  $16^3$  and densities  $\rho = 0.52, 0.53, 0.54, 0.55, 0.56, 0.57, 0.58, 0.59, 0.60, 0.61$  (from Ref. [36]).

where the average  $\langle \cdots \rangle$  is performed over the time t'. In Fig. 3, we show the relaxation functions of the self-overlap (17), for a system of size  $16^3$ , for various densities between  $\rho$ =0.52 and 0.61. Observe that for high density, the relaxation functions clearly develop a two step relaxation, signaling the existence of two well separated time scales in the system. The first short time decay of the relaxation functions can be interpreted as due to the motion of the particles in the quasi-frozen environment, which on this time scales appear as quenched, while the second decay is due to the evolution of environment. The form of the relaxation in Fig. 3 can be well fitted with the functional form predicted by the mode coupling theory.

In Fig. 4, we show the dynamical non-linear susceptibility (18) for different values of the density. It has the same behaviour of the p-spin model in mean field and of the molecular dynamics simulation of the Lennard–Jones binary mixture [38], namely a maximum  $\chi(t^*)$  that seems to diverge together with the time of the maximum  $t^*$ , when the density grows. Comparing these results to those obtained in the model with quenched interactions, we conclude that the critical behaviour of the dynamical susceptibility is reminiscent of the thermodynamic transition present in the quenched model, and signaled by the divergence of the static non-linear susceptibility, therefore, suggesting a similar mechanism also in supercooled glass-forming liquids.

#### 8. Percolation in phase space

The FP model may give some indication of the behaviour of glassy systems in phase space. In Fig. 5, the mean square displacement for the frustrated lattice gas model is reported with quenched interactions  $\langle \Delta r^2 \rangle = \langle (r(t) - r(0))^2 \rangle$  where r(t) is a vector

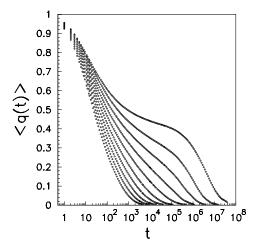


Fig. 4. Dynamical susceptibility in the annealed model, for the same system size and densities of Fig. 3 (from Ref. [36]).

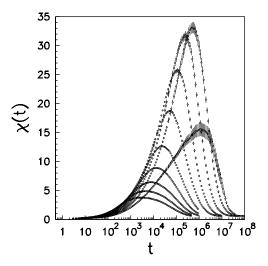


Fig. 5. Mean square displacement in the site FP model as a function of time on a square lattice with L=32, for densities (from upper curves to lower ones):  $\rho=0.452, 0.586, 0.730, 0.756, 0.766, 0.777, 0.784, 0.785, 0.787$  (after Ref. [29]).

whose coordinates coincide with the coordinates of all the particles, at time t. At low density, the curves show a linear behaviour, which corresponds to normal diffusion. As the density increases, the mean square displacement shows first a shoulder and then a plateau corresponding to the localization of particles (as in some molecular dynamic simulations of supercooled glass forming liquids, see Refs. [40,41]).

The vector r(t) can also be interpreted as the position in phase space of the point representing the microscopic state of the system. Due to frustration, there are many points in phase space which are not allowed. These points correspond to those configurations which contain at least one frustrated loop. The evolution in time of the state correspond to a trajectory in such space. As the density of particles increases, the allowed phase space gets reduced until a critical density is reached below which the phase space becomes disconnected and the point in phase space gets localized. This localization problem can be seen like a percolation process in phase space. In this percolation problem, the connectivity is fixed by the dynamics. For example, for a diffusive dynamics the representative point in phase space moves in one step to the nearest neighbour. But if the dynamics allows to exchange a particle with a hole at large distances, the representative point can jump to farther nearest neighbours. Therefore, the connected regions depend on the particular dynamics. A similar picture based on a percolation process in phase space was originally proposed by Campbell [42], for spin glasses and glasses. Here the site FP model reproduce exactly such picture since in a jump from one allowed configuration to another, there are no energy barrier to overcome. However, the points in phase space not allowed are not randomly distributed as in random percolation.

#### 9. Conclusions

In conclusion, I have presented the properties of the FP model. This is a generic model which may be relevant to many systems where the concept of frustration and connectivity plays a major role. In fact while the bond FP maps exactly on the SG model, the site FP has been shown to be relevant to other systems like supercooled liquids and granular materials [43] where frustration plays a major role.

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