LETTER

Long-range frustration in $T = 0$
first-step replica-symmetry-broken
solutions of finite-connectivity
spin glasses

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Abstract. In a finite-connectivity spin glass at the zero-temperature limit,
long-range correlations exist among the unfrozen vertices (whose spin values
are non-fixed). Such long-range frustrations are partially removed through the
first-step replica-symmetry-broken (1RSB) cavity theory, but residual long-range
frustrations may still persist in this mean-field solution. By way of population
dynamics, here we perform a perturbation–percolation analysis to calculate the
magnitude of long-range frustrations in the 1RSB solution of a given spin-glass
system. We study two well-studied model systems, the minimal vertex-cover
problem and the maximal 2-satisfiability problem. This work points to a possible
way of improving the zero-temperature 1RSB mean-field theory of spin glasses.

Keywords: cavity and replica method, ergodicity breaking (theory), spin glasses
(theory), message-passing algorithms

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Spin glasses are simple models for a large class of disordered systems with quenched randomness and frustration [1]. At low temperatures, ergodicity is broken in a spin-glass system, whose configurational phase space splits into exponentially many ergodic domains, each of which corresponds to a thermodynamic state. Within each thermodynamic state, a vertex’s spin is partially frozen, but the preferred spin orientation and the degree of preference are vertex-dependent. Mean-field theories for spin glasses on random graphs of finite connectivity [2,3] have attracted a lot of research interest in recent years. The work of M´ezard and Parisi [3] combines the classical Bethe–Peierls approximation (BA) [4] with the exponential proliferation of thermodynamic states. It is a first-step replica-symmetry-broken (1RSB) cavity solution for finite-connectivity spin glasses [3]. The zero-temperature limit of this mean-field theory [5] has found important applications in computer science and information theory [6,7].

The essence of the BA is assuming statistical independence among the vertices in the nearest-neighbour set $\partial_i$ of any given vertex $i$ in the cavity graph where $i$ is removed. Very recently, the cavity approximation and loop expansion method [8]–[11] were developed, which calculate the statistical correlations among cavity vertices in $\partial_i$. These approaches at the present stage work only in the ergodic high-temperature paramagnetic phase. Another theoretical approach of going beyond the BA, which works in the spin-glass phase at the other limit of temperature $T \to 0$ [12,13], is to consider long-range frustrations among the unfrozen cavity vertices in the set $\partial_i$. At the $T \to 0$ limit, a vertex $i$ of a spin-glass system either takes the same spin value in all the relevant configurations which contribute to the free energy of the system, or is unfrozen and takes different spin values in different configurations. With respect to a pre-specified value $\sigma^* \in \pm 1$, an unfrozen vertex $i$ may be type-I or type-II unfrozen, depending on whether or not the fixation of $\sigma_i$ to $\sigma_i = \sigma^*$ leads to the fixation of the spin values of a finite fraction of all the other unfrozen vertices [12,13]. All the type-I unfrozen vertices in a spin-glass system are strongly correlated, no matter how far apart they are separated from each other. Such strong correlations are referred to as long-range frustrations.

The present work represents a first step in the on-going effort of integrating the physical idea of long-range frustration into the 1RSB mean-field cavity approach of spin glasses. Long-range frustration is associated with ergodicity breaking: type-I unfrozen vertices are absent in the paramagnetic phase. Even in the spin-glass phase, long-range frustration should vanish within each ergodic subdomain of the configurational space. However, the configurational space of a spin-glass system may be organized to be far more complex than what is assumed in the 1RSB mean-field theory [5]. For example, a macroscopic state of the 1RSB solution may actually be a merge of several true thermodynamic states (referred to as the second kind or type II instabilities in [14] and [15]). Therefore, it may be possible that type-I unfrozen vertices still exist within a macroscopic state of the 1RSB mean-field solution. Here this possibility is checked by a quantitative percolation analysis (by population dynamics) of spin-flip perturbations. We work on two concrete models, the minimal vertex-cover problem [16] and the maximal 2-satisfiability problem [17]; we find that residual long-range frustrations exist in the former system but are absent in the latter system. This work suggests a possible way of improving the zero-temperature 1RSB mean-field theory of spin glasses. We also discuss possible other extensions of the present theoretical framework. The existence of residual long-range frustrations is a signature of the instability of the $T = 0$ 1RSB mean-field theory.
solution toward further steps of replica-symmetry-breaking [14, 15, 18, 19]. It is not clear, however, whether the onset of long-range frustration is a necessary condition for the 1RSB macroscopic state to be non-ergodic (i.e. made of smaller sub-states).

**Percolation analysis.** Type-I unfrozen vertices form a giant cluster in a graph, their existence therefore can be detected by a percolation analysis. (The propagation of correlations among type-I unfrozen variables is close in spirit to the notion of bug proliferation of [20].) To introduce the basic methodology of percolation analysis by population dynamics, let us as an example calculate the fraction \( q \) of vertices that are in the giant component of a random Poissonian graph of mean vertex-degree \( c \) [21]. We note that a vertex \( i \) is in the giant component if at least one vertex in its nearest-neighbour set \( \partial i \) is in the giant component of the cavity graph where \( i \) is removed. We construct a population of binary elements, each of which is either 1 (in the giant component) or 0 (not in the giant component). At each elementary update, \( k \) elements are randomly chosen from the population (\( k \) being a random integer governed by the Poisson distribution of mean \( c \)); then a randomly chosen element of the population is set to be 0 if all these \( k \) (input) elements are zero, otherwise it is set to be 1. The giant component size \( q \) is estimated to be the fraction of 1’s in the whole population. We found that this value is identical to the value predicted by the well-known formula \( q = 1 - e^{-cq} \) [21]. In what follows we analyse long-range frustrations in spin glasses using this methodology. We demonstrate our approach by first working on the minimal vertex-cover problem.

**The minimal vertex-cover.** For a given graph \( G \) of \( N \) vertices and \( M \) edges \((i, j)\) between pairs of vertices \( i \) and \( j \), a minimal vertex-cover is a spin pattern \( \{\sigma_i \in \pm 1\} \) which satisfies the constraint

\[
\prod_{(i,j) \in G} \left[ 1 - \frac{(1 + \sigma_i)(1 + \sigma_j)}{4} \right] \equiv 1, \tag{1}
\]

and which minimizes the total energy

\[
E(\sigma_1, \ldots, \sigma_N) = \sum_{i=1}^{N} \frac{1 - \sigma_i}{2}. \tag{2}
\]

A minimal vertex-cover for a given graph \( G \) is a spin pattern with the maximal number of uncovered (+1) vertices, while for each edge of the graph at least one of its two end vertices is covered (\( \sigma = -1 \)). The mean-field 1RSB cavity solution of the minimal vertex-cover problem on finite-connectivity random graphs was reported in [22]. When the mean vertex degree \( c \) of the random graph satisfies \( c > 2.7183 \), the system is in the spin-glass phase. In this spin-glass phase, the 1RSB theory assumes that, in the limit of graph size \( N \to \infty \), there are exponentially many local optimal vertex covers for the constrained system. Each local optimal pattern is stable with respect to any perturbation which flips a finite number of spins. A macroscopic state \( \alpha \) of the 1RSB mean-field solution contains a set of local optimal patterns of the same energy \( E_\alpha \). Two patterns in the same macroscopic state are assumed to be similar to each other. At \( T = 0 \), the total grand free energy \( G \) of the system can be defined by the equation

\[
\exp(-yG) = \sum_\alpha \exp(-yE_\alpha), \tag{3}
\]
where the summation is over all the macroscopic states of the system; $y$ is a re-weighting parameter [5], whose value is chosen such that $G(y)$ attains maximality [23].

A vertex $i$ is referred to as being positively (negatively) frozen in macroscopic state $\alpha$ if its spin value is positive (negative) in all the configurations of this macroscopic state. This spin value freezing is caused by energy minimization under the constraint equation (1). Vertex $i$ is said to be unfrozen in macroscopic state $\alpha$ if it is neither positively nor negatively frozen. If in the cavity graph $G \setminus i$ all the vertices in the nearest-neighbour set $\partial i$ of vertex $i$ are negatively frozen in state $\alpha$, then $i$ will be positively frozen in macroscopic state $\alpha$ of the full graph $G$; on the other hand, if two or more vertices in $\partial i$ are positively frozen in state $\alpha$ of $G \setminus i$, then $i$ will be negatively frozen in state $\alpha$ of $G$. However, the remaining situations are tricky. As an example, consider the case in which two (say $j$ and $k$) or more of these vertices are type-I unfrozen (with respect to the minus spin value, of course), it may be that flipping $\sigma_j$ to $\sigma_j = -1$ will force the spin of vertex $k$ to be $\sigma_k = +1$! This is because when a type-I unfrozen vertex $j$ is fixed to $\sigma_j = -1$, eventually a percolating cluster of other unfrozen vertices in the whole system will also have their spins be fixed (either positively or negatively); all the other type-I unfrozen vertices are in this giant cluster [12].

In the mean-field 1RSB cavity solution [22] all the unfrozen vertices are assumed to be type-II, and no long-range frustration effect is considered. Here let us assume that initially some of the vertices in each macroscopic state are type-I unfrozen. We will then check whether the fraction of type-I unfrozen vertices will shrink to zero in the 1RSB population dynamics. We will focus on whether type-I unfrozen vertices persist but not on their energetic effects. In other words, we assume that the type-I unfrozen cavity vertices in the nearest-neighbour set $\partial i$ of each vertex $i$ can take the minus spin value simultaneously. Under this simplification, let us consider a cavity vertex $j$ which is connected by an edge $(i, j)$ to a vertex $i$ of the graph $G$. In the cavity graph $G \setminus i$ in which vertex $i$ is being removed, the cavity vertex $j$ will be type-I unfrozen if: (1) only one of the vertices (say $k$) in the set $\partial j \setminus i$ is positively frozen in the graph $G \setminus i, j$, and (2) this vertex $k$ is itself connected to one or more type-I unfrozen vertices of the cavity graph $G \setminus i, j, k$ [12]. Let us denote by $\hat{\pi}_{j-i}^0$ the fraction of macroscopic states in which vertex $j$ is positively frozen and none of its nearest neighbours is type-I unfrozen in the cavity graph $G \setminus i, j$. Similarly, $\hat{\pi}_{j-i}^0$, is the fraction of states in which $j$ is positively frozen and some of its nearest neighbours is type-I unfrozen in $G \setminus i, j$; $\hat{\pi}_{j-i}^*$ is the fraction of states in which $j$ is type-II unfrozen in graph $G \setminus i$; and $\hat{\pi}_{j-i}^*$ is the fraction of states in which $j$ is type-I unfrozen in graph $G \setminus i$. Following the 1RSB cavity approach [22] we can write down the following iterative equations for a Poissonian random graph:

$$
\hat{\pi}_{j-i}^0 = \frac{\prod_{k \in \partial j \setminus i}[1 - \hat{\pi}_{k-j}^0 - \hat{\pi}_{k-j}^* - \hat{\pi}_{k-j}^0]}{e^{-y} + (1 - e^{-y}) \prod_{k \in \partial j \setminus i}[1 - \hat{\pi}_{k-j}^0 - \hat{\pi}_{k-j}^*]}
$$

$$
\hat{\pi}_{j-i}^* = \frac{\prod_{k \in \partial j \setminus i}[1 - \hat{\pi}_{k-j}^0 - \hat{\pi}_{k-j}^*] \prod_{k \in \partial j \setminus i}[1 - \hat{\pi}_{k-j}^0 - \hat{\pi}_{k-j}^*]}{e^{-y} + (1 - e^{-y}) \prod_{k \in \partial j \setminus i}[1 - \hat{\pi}_{k-j}^0 - \hat{\pi}_{k-j}^*]}
$$
Replica-symmetry-broken solutions of finite-connectivity spin glasses

$$\hat{\pi}^*_j \rightarrow i = \frac{e^{-y} \sum_{k \in \partial j \setminus i} \hat{\pi}^0_{k \rightarrow j} \prod_{l \in \partial j \setminus i \setminus k} [1 - \hat{\pi}^0_{l \rightarrow j} - \hat{\pi}^0_{i \rightarrow l}]}{e^{-y} + (1 - e^{-y}) \prod_{k \in \partial j \setminus i} [1 - \hat{\pi}^0_{k \rightarrow j} - \hat{\pi}^0_{i \rightarrow j}]}.$$  

$$\tilde{\pi}^*_{j \rightarrow i} = \frac{e^{-y} \sum_{k \in \partial j \setminus i} \tilde{\pi}^0_{k \rightarrow j} \prod_{l \in \partial j \setminus i \setminus k} [1 - \tilde{\pi}^0_{l \rightarrow j} - \tilde{\pi}^0_{i \rightarrow l}]}{e^{-y} + (1 - e^{-y}) \prod_{k \in \partial j \setminus i} [1 - \tilde{\pi}^0_{k \rightarrow j} - \tilde{\pi}^0_{i \rightarrow j}]}.$$  

Equation (4)

Two steady-state distributions $P(\hat{\pi}^0_{j \rightarrow i}, \tilde{\pi}^0_{j \rightarrow i}, \hat{\pi}^*_{j \rightarrow i}, \tilde{\pi}^*_{j \rightarrow i})$ and $P(\hat{\pi}^0_{i \rightarrow j}, \tilde{\pi}^0_{i \rightarrow j}, \hat{\pi}^*_{i \rightarrow j}, \tilde{\pi}^*_{i \rightarrow j})$ on all edges $(i, j)$ of the graph can be obtained by population dynamics simulations [22]. An array of $N = 10^6$ vectors $\pi_{j \rightarrow i} = \{\hat{\pi}^0_{j \rightarrow i}, \tilde{\pi}^0_{j \rightarrow i}, \hat{\pi}^*_{j \rightarrow i}, \tilde{\pi}^*_{j \rightarrow i}\}$ is constructed; elements of this array are then updated according to equation (4). At the given value of the re-weighting parameter $y$ the grand free-energy density of the system is calculated [22], as well as the following long-range order parameter $R_{j \rightarrow i}$ for each directed edge $j \rightarrow i$:

$$R_{j \rightarrow i} \equiv \frac{\tilde{\pi}^*_{j \rightarrow i}}{(\tilde{\pi}^*_{j \rightarrow i} + \hat{\pi}^*_{j \rightarrow i})}.$$  

Equation (5)

$R_{j \rightarrow i}$ measures the probability of an unfrozen cavity vertex $j$ being actually type-I unfrozen.

For an ensemble of random Poissonian graph with mean vertex degree $c = 10$, the population dynamics results are shown in figure 1. At $y = y^* = 3.130(8)$ the grand free-energy density reaches maximum, which corresponds to the ground-state energy density of the system. The mean long-range frustration order parameter $R = (1/N) \sum R_{j \rightarrow i}$ decreases with the re-weighting parameter $y$ and becomes zero for $y > 3.25$. Most importantly, at $y = y^*$ the value of $R$ is positive ($R = 0.0534$). Figure 1(B) shows the distribution of the $R_{j \rightarrow i}$ values at $y = y^*$. This distribution has a peak at $R_{j \rightarrow i} = 0$ and another peak at $R_{j \rightarrow i} \approx 0.043$. On average an unfrozen vertex is type-I unfrozen in about five percent of the macroscopic states. We therefore conclude that in the 1RSB mean-field treatment of the minimal vertex-cover problem there still exist residual long-range frustrations. We have also checked that the above qualitative conclusion holds also for other values the mean vertex degrees $c > 2.7183$. For example, at $c = 5$, the mean long-range frustration order parameter is $R = 0.0405$, slightly below the value for $c = 10$.

Does long-range frustration exist in the 1RSB mean-field cavity solutions of all finite-connectivity spin-glass models with two-body interactions? The following example suggests that this is not necessarily true.

The maximal 2-satisfiability problem. On a random factor graph [24] $G$ with $N$ variable nodes $i$ and $M = \alpha N$ function nodes $a$, each of which connects to two randomly chosen variable nodes $i$ and $j$, the 2-SAT energy function is defined as

$$E(\sigma_1, \ldots, \sigma_N) = \sum_{a \in G} \frac{(1 - J^a_{i} \sigma_i)(1 - J^a_{j} \sigma_j)}{4}.$$  

Equation (6)

In equation (6) the quenched coupling constant $J^a_{i}$ of the edge between the function node $a$ and variable node $i$ is equal to $+1$ or $-1$ with equal probability. The Max-2SAT problem consists of finding a binary spin pattern which minimizes the configurational energy equation (6). For a random factor graph, it is well known that the ground-state energy of the system is zero when $\alpha < 1$ [17]; it becomes positive for $\alpha > 1$, and long-range frustration builds up in the Max-2SAT when $\alpha > 4.4588$ [13].

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We have applied the perturbation–percolation analysis on the 1RSB solution of the Max-2SAT problem defined on an ensemble of random factor graphs of $\alpha = 10$. As shown in figure 2, the grand free-energy density of the system reaches maximality at $y = 1.932$, but the mean long-range frustration order parameter $R$ already drops to zero at $y \approx 0.75$. (For $\alpha = 20$ similar results are obtained.) Consequently, the present percolation analysis suggests that the 1RSB mean-field solution of the Max-2SAT problem is free of any residual long-range frustrations. Whether or not long-range frustrations persist in the mean-field 1RSB solution therefore also depends on the particular system under study.

In passing we note that the 1RSB mean-field theory reports a ground-state energy density of $1.307040(2)$. Interestingly, this value is just located at the middle between the predicted lower and upper bound of $1.301378$ and $1.311933$ [13].
Conclusion and discussion. In summary, in this paper we have investigated by population dynamics the possibility of long-range correlations among the unfrozen vertices in the zero-temperature first-step replica-symmetry-breaking solutions of finite-connectivity spin glasses. The perturbation–percolation analysis of this work demonstrated that residual long-range frustrations may still persist in the mean-field 1RSB cavity solutions. The present theoretical approach is also able to give a quantitative estimate of the magnitude of long-range frustrations in the 1RSB mean-field theory.

At the present stage we are interested in the existence or not of type-I unfrozen vertices in the 1RSB mean-field theory. We have not yet actually calculated the energetic effects of type-I unfrozen vertices. We hope to return to this point in later publications. If the mean long-range frustration order parameter is positive, energetic effects of long-range frustrations can be included into the present population dynamics approach, and a better estimate of the ground-state energy density can be obtained. In the minimal vertex-cover problem, given the fact that the mean long-range frustration order parameter $R$ is of the order of $10^{-2}$ in the 1RSB solution, the correction to the ground-state energy of the system might turn out to be very small.

The presence of long-range correlations may reflect the instability of the 1RSB mean-field solution. Each macroscopic state of the 1RSB solution may be non-ergodic and can be further divided into a group of sub-states. A procedure of stability analysis for zero-temperature 1RSB mean-field solutions has been outlined in [14,15]. It is of interest to apply this analysis to spin-glass problems with two-body interactions and check whether or not its qualitative conclusions are consistent with the results obtained by the long-range frustration analysis. The estimated mean long-range frustration value $R$ should depend on the type of ansatz (1RSB, 2RSB, . . .) used for the computation. When a macroscopic state of the 1RSB solution further breaks into sub-macroscopic states (2RSB), a type-I unfrozen vertex in the macroscopic state of the 1RSB solution may become frozen in the daughter sub-macroscopic states of the 2RSB solution. The mean long-range frustration

Figure 2. Grand free energy density (circles) and mean long-range frustration $R$ (squares) for the random 2-SAT problem with $\alpha = 10$. The vertical dotted line indicates the point of $y = 1.932$. 
value $R$ therefore will decreases as higher steps of RSB are assumed. The present work also suggested that, for some spin-glass systems, long-range frustrations may be absent in the 1RSB mean-field cavity solutions. For these systems, maybe the mean-field 1RSB cavity theory is already enough to describe their equilibrium properties at temperature $T \to 0$. Higher levels of replica-symmetry-breaking may not be needed any more. However, it is not known whether the existence of long-range frustration is a necessary condition for the zero-temperature 1RSB mean-field solution to be unstable. This point should be checked seriously.

Both the earlier [12, 13] and the present work study the statistical mechanical properties of finite-connectivity spin glasses at the limit of zero temperature. When the temperature $T$ is low but still positive, long-range correlations may also exist in mean-field solutions of spin-glass systems. However, at finite temperatures we cannot make the distinction between frozen and unfrozen vertices. This is because all the vertices are unfrozen. How to extend the present theoretical approach to the case of positive temperatures is an interesting and challenging problem.

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