

From one solution of a 3-satisfiability formula to a solution cluster: Frozen variables and entropy

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A solution to a 3-satisfiability (3-SAT) formula can be expanded into a cluster, all other solutions of which are reachable from this one through a sequence of single-spin flips. Some variables in the solution cluster are frozen to the same spin values by one of two different mechanisms: frozen-core formation and long-range frustrations. While frozen cores are identified by a local whitening algorithm, long-range frustrations are very difficult to trace, and they make an entropic belief-propagation (BP) algorithm fail to converge. For the BP algorithm to reach a fixed point, the spin values of a tiny fraction of variables (chosen according to the whitening algorithm) are externally fixed during the iteration. From the calculated entropy values, we infer that, for a large random 3-SAT formula with constraint density close to the satisfiability threshold, the solutions obtained by the survey-propagation or WALKSAT algorithms belong neither to the most dominating clusters of the formula nor to the most abundant clusters. This work indicates that a single-solution cluster of a random 3-SAT formula may have further community structures.

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I. INTRODUCTION

The K -satisfiability (K -SAT) problem is a prototypical constraint satisfaction problem in the nondeterministic polynomial complete (NP-complete) complexity class [1]. Statistical physicists became interested in this computer science problem since the discovery of phase-transition phenomena in the ensemble of random 3-SAT formulas in the early 1990s. Randomly generated 3-SAT formulas were found to be either almost always satisfiable or almost always unsatisfiable depending on whether or not the density of constraint α [defined by Eq. (3) below] is lower than a critical value α_s (the SAT-UNSAT transition point) [2,3]. Furthermore, random 3-SAT formulas whose satisfiability being most difficult to resolve all have constraint densities close to the critical value α_s [2]. A lot of theoretical work (see, e.g., Refs. [4–14]) has been done to understand the satisfiability transition in the random K -SAT problem and the rapid increase of resolution time as the constraint density α approaches α_s .

In the SAT phase with constraint density α close to α_s , the solution space of a typical large random K -SAT formula ($K \geq 3$) can be grouped into many clusters. The solution clusters are not homogeneous in size; some clusters may contain many more solutions than others. Therefore the solution clusters are characterized by a (continuous or discontinuous) spectrum of entropy densities [13–15]. On the other hand, it is not clear whether different solution clusters are separated by high-energy barriers or they can be reached one from the other through paths of low-energy intermediate partial solutions. This is one of the major open questions concerning the organization of the solution space of a random K -SAT formulas. In this connection, it was recently realized that clustering of the solution space in the random K -SAT problem does not pose real difficulty for heuristic local search algorithms [16–20]. Algorithms such as GSAT, WALKSAT, and CHAINSAT [16,18,19] appear to be capable of efficiently escaping from valleys in the energy landscape of a random K -SAT formula. These experimental experiences led to the conjecture that what really makes finding a satisfying solu-

tion hard is the presence of frozen variables (see, e.g., Ref. [21] and more recent papers [18,22–24]). A frozen variable in a solution cluster is a variable which is the same literally in all solutions of the cluster. If a finite fraction of variables are frozen in a given solution cluster, it was argued that it would be difficult for a local algorithm to assign values to all these variables and that such solutions would be hard to find [25,26]. The freezing transition for the random K -SAT problem in principle can be estimated by the entropic cavity method of statistical mechanics [27], but extensive mean-field population dynamics simulations [13–15] are needed. For the random 3-SAT problem the known quantitative estimation of the freezing transition point comes from a finite-size scaling analysis on exact enumeration results [23].

Earlier mean-field theoretical studies [12–14] on the K -SAT problem have focused on ensemble-averaged properties. In this work, we take a complementary approach and investigate the properties of solution clusters that are associated with single-reference solutions. This study has been driven by two main motivations: First, we wish to know in more detail the “local structures” of the solution space of the random 3-SAT problem, which might be invisible in ensemble studies; and second, we wish to know whether the solutions obtained by the survey-propagation and WALKSAT algorithms for a given random 3-SAT formula are contained in the dominating solution clusters of this formula. Given an initial satisfying solution for a 3-SAT formula, we use the whitening algorithm of Parisi [28] (see also Refs. [18,29]) to determine which variables are frozen (i.e., taking the same spin value) in the associated solution cluster. A simple mean-field formula [Eq. (5)] is also given, which predicts with high precision the fraction of frozen variables in planted solutions for the type-B random 3-SAT formulas studied in this paper. We point out that, even if a reference solution can be completely whitened by the whitening algorithm, some variables in the associated solution cluster may still be frozen. This is because variable freezing can be caused by another independent mechanism: namely, long-range frustration among unfrozen variables as discussed in Refs. [30,31]. When the neighboring unfrozen variables of a variable i are long-

rangely frustrated, this variable very probably will be frozen. Two heuristic algorithms are constructed to identify variables that are frozen due to long-range frustrations. The entropy of the solution cluster associated with a given reference solution is calculated by the entropic cavity method, taking the reference solution as initial condition for the set of zero-energy belief-propagation (BP) iterative equations [Eqs. (9) and (11)]. The entropy values reported in this paper are consistent with the mean-field results of Ref. [14].

For large random 3-SAT formulas with constraint densities close to α_c , we find that if solutions obtained by the survey-propagation (SP) [8,9,32], the WALKSAT [17], or the belief-propagation-guided decimation [12,20] algorithms are used as initial conditions, the entropic BP algorithm *always* fails to reach a fixed point. Besides the ensemble of completely random 3-SAT formulas, a set of large random 3-SAT formulas containing a prespecified satisfying solution are also studied, and for each of them several additional solutions are obtained by the SP and WALKSAT algorithms. For a 3-SAT formula in this second ensemble, if the entropic BP iterative equations are run with the planted solution as the initial condition, a fixed point is quickly reached, but if a solution obtained by the SP or the WALKSAT algorithm is used as the initial condition, the iterative equations again fails to converge. This observation suggests that planted solutions and solutions obtained by the SP algorithm are quite different. In cases when the BP algorithm fail to reach a fixed point, we fix the spin values of a tiny fraction of variables and then re-run the BP iteration equations. The modified BP iteration process will converge if this set of externally fixed variables are chosen according to the outcome of the whitening program.

In the remaining part of the paper we work exclusively on the random 3-SAT problem, but the illustrated approach should be directly applicable to more general cases. The following section list the ensembles of random 3-SAT formulas used in this work. In Sec. III we investigate the whitening algorithm and present a mean-field formula to describe the freezing transition in a cluster of solutions. And the SPINFLIP algorithm and another heuristic search algorithm are introduced to search for frozen variables in a completely white solution. The entropy of the solution cluster associated with a planted solution is calculated by the entropic BP algorithm in Sec. IV. For solution clusters associated with single SP or WALKSAT solutions, their entropy values and fraction of frozen variables are calculated in Sec. V by combining BP with the whitening program. We conclude this work in Sec. VI.

II. GENERATION OF SATISFIABLE RANDOM 3-SAT FORMULAS

A K -SAT formula contains N variables and M constraints (clauses). Each of the N variables (i, j, k, \dots) has a binary spin state $\sigma_i \in \{-1, +1\}$. Each of the M constraints (a, b, c, \dots) involves K different variables ($i_a^1, i_a^2, \dots, i_a^K$) and prohibits these variables from taking a specified pattern $(-J_a^1, -J_a^2, \dots, -J_a^K)$, out of the total number of 2^K possible spin patterns of length K . An energy function can be defined for a given K -SAT formula as

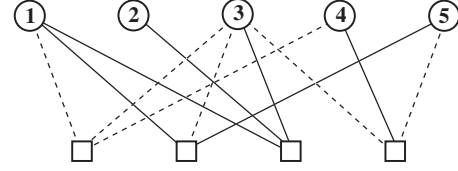


FIG. 1. Factor-graph representation for a simple 3-SAT formula with energy expression $H=(1+\sigma_1)(1+\sigma_3)(1+\sigma_4)/8+(1-\sigma_1)(1+\sigma_3)(1-\sigma_5)/8+(1-\sigma_1)(1-\sigma_2)(1-\sigma_3)/8+(1+\sigma_3)(1-\sigma_4)(1+\sigma_5)/8$.

$$E(\sigma_1, \sigma_2, \dots, \sigma_N) = \sum_{a=1}^M \prod_{i \in \partial a} \left(\frac{1 - J_a^i \sigma_i}{2} \right), \quad (1)$$

where ∂a means the set of variables involved in constraint a . For a given spin configuration $\vec{\sigma} \equiv \{\sigma_1, \sigma_2, \dots, \sigma_N\}$, the energy $E(\vec{\sigma})$ is equal to the number of unsatisfied clauses. The zero-energy configurations (if they exist) of Eq. (1) correspond to the solutions of the K -SAT formula. A K -SAT formula has a convenient factor graph representation (see the example shown in Fig. 1): variables are denoted by circular nodes and constraints by square nodes, and there is an edge between a constraint node a and a variable node i if and only if variable i participates in constraint a . The edge (a, i) is solid if $J_a^i = 1$ and is dashed if $J_a^i = -1$.

In the present paper, we focus on random K -SAT formulas with $K=3$. To generate a random 3-SAT formula, M different triplets (i, j, k) are randomly chosen from the total number of $N(N-1)(N-2)/6$ possible triplets of variable nodes. A constraint a is applied on each selected triplet (i, j, k) , and it prohibits the simultaneous spin assignment $(\sigma_i = -J_a^i) \wedge (\sigma_j = -J_a^j) \wedge (\sigma_k = -J_a^k)$, where \wedge means logical AND. We use two different ways to generate the prohibited patterns $(-J_a^i, -J_a^j, -J_a^k)$ for the M constraints, which we call the type-A and type-B formulas (see below). For a given satisfiable 3-SAT formula, let us denote a particular solution as $\vec{\sigma}^* \equiv \{\sigma_1^*, \sigma_2^*, \dots, \sigma_N^*\}$. Since $\vec{\sigma}^*$ is compatible with all the constraints of the formula, for each constraint a the associated edge vector

$$\tilde{J}_a \equiv (J_a^i \sigma_i^*, J_a^j \sigma_j^*, J_a^k \sigma_k^*) \quad (i, j, k \in \partial a) \quad (2)$$

can have at most two negative elements. The clauses of the 3-SAT formula can therefore be grouped into three types with respect to the reference solution $\vec{\sigma}^*$, and we denote by q_0 , $3q_1$, and $3q_2$, respectively, the fraction of constraints a whose edge vector \tilde{J}_a have zero, one, and two negative elements. Obviously,

$$q_0 + 3q_1 + 3q_2 \equiv 1.$$

For the first ensemble of random formulas used in this paper (type-A formulas), the prohibited spin pattern $(-J_a^i, -J_a^j, -J_a^k)$ of each clause a is independently and uniformly randomly chosen from the total number of eight possibilities. Such random formulas are satisfiable with a high probability as long as the constraint density α defined by

$$\alpha \equiv M/N \quad (3)$$

is less than 4.267 [8,9]. For each constraint density $\alpha \in \{4.20, 4.21, 4.22, 4.23, 4.24, 4.25\}$, we generate a set of random 3-SAT formulas of $N=10^6$ variables; for each of these formulas, we use the survey-propagation algorithm [9,32] (downloaded from Riccardo Zecchina's webpage) to obtain five different satisfying solutions. For $\alpha=4.20$ we also use the WALKSAT algorithm [17] (version 45, downloaded from the WALKSAT homepage) with optimized noise parameter ($p=0.57$ [18]) to obtain another set of solutions. The solutions serve as initial conditions for the whitening and the belief-propagation simulations of the next two sections. For the benefit of later discussions, we refer to a solution obtained by the SP algorithm as an SP solution and a solution obtained by WALKSAT as a WALKSAT solution.

The second ensemble of satisfiable random formulas (type-B formulas) used in this paper are constructed in such a way that a pre-given spin configuration $\vec{\sigma}^*$ is a solution. Such ensembles with planted solutions were investigated in the literature earlier [33] and are known to have different properties from standard random K -satisfiability; see, e.g., [34,35]. For each constraint a of the formula, the value of its edge vector \vec{J}_a as defined by Eq. (2) is assigned according to the following rule [33]: a uniformly distributed random variable $r \in [0,1)$ is first generated; if $r \leq q_0$, then \vec{J}_a is set to be $(+1, +1, +1)$; if $q_0 < r \leq q_0 + 3q_1$, then \vec{J}_a is chosen uniformly randomly from the set $\{(+1, +1, -1), (+1, -1, +1), (-1, +1, +1)\}$; otherwise, \vec{J}_a is chosen uniformly randomly from the set $\{(+1, -1, -1), (-1, +1, -1), (-1, -1, +1)\}$. For simplicity and without loss of generality, in this paper we set the pre-given spin configuration to be $\vec{\sigma}^* = (+1, +1, \dots, +1)$ when constructing type-B random 3-SAT formulas.

III. FREEZING OF VARIABLES IN A SOLUTION CLUSTER: TWO DIFFERENT MECHANISMS

Starting from a given solution $\vec{\sigma}^*$ of a satisfiable 3-SAT formula F , one can (in principle) build a connected network of solutions which contains as many solutions of formula F as possible. In this solution cluster, two solutions $\vec{\sigma}^1$ and $\vec{\sigma}^2$ are regarded as being directly connected if and only if they differ in the spin value of a single variable. From one solution of the cluster, one can reach any another solution of the same cluster by a sequence of single-spin flips (within the whole solution space of formula F). We refer to such a connected network of solutions as a solution cluster (or simply cluster) for formula F . The spin states of some variables of the formula may take the same value in all the solutions of the cluster. Such variables are referred to as frozen variables; they are strongly constrained in the solution cluster.

There are two different mechanisms which cause freezing of variables in a solution cluster. The first mechanism, which we refer to as “frozen-core formation,” can be described using the following whitening process [28]. Starting from a given reference solution $\vec{\sigma}^*$ of a K -SAT formula, at step 0 of the whitening process, all the clauses a that are simulta-

neously satisfied by at least two variables of solution $\vec{\sigma}^*$ are marked as white and all the variables that do not satisfy any clause or satisfy only white clauses are marked as white, while the remaining clauses and variables are all marked as nonwhite. Then at each following step t of the whitening process (i) all the nonwhite clauses which are connected to at least one white variables are marked as white, and then (ii) all the nonwhite variables which satisfy only white clauses are marked as white. The whitening process stops at step $t \geq 1$ if the number of newly whitened clauses (and variables) is zero. After this whitening process has finished, if a variable i is left as being nonwhite, one can prove that it is impossible to travel from $\vec{\sigma}^*$ to another satisfying configuration with $\sigma_i = -\sigma_i^*$ using only satisfying single-spin flips [36]. In other words, the spin of a nonwhite variable node i is frozen to σ_i^* . The set of nonwhite variables in the reference solution $\vec{\sigma}^*$ forms one or several frozen cores. For a variable i in such a frozen core, there exists at least a clause a of the formula that is satisfied only by variable i in the configuration $\vec{\sigma}^*$ and that is either not connected to other variables or is connected only to other variables belonging to the same frozen core of i . As the constraint density α increases, the freezing of variables due to frozen-core formations is therefore a phenomenon of bootstrap percolation.

The final result of the whitening process actually is independent of the order in which the variables are being whitened [28]. It then follows that, in a solution cluster of a K -SAT problem, if one of the solutions can be completely whitened, then all the other solutions can also be completely whitened. To prove this, let us suppose the contrary could be true; i.e., there exist two solutions of the same cluster, $\vec{\sigma}^1$ and $\vec{\sigma}^2$, where $\vec{\sigma}^1$ can be completely whitened and $\vec{\sigma}^2$ contains a nonempty set A of nonwhite variables. One can change $\vec{\sigma}^2$ into $\vec{\sigma}^1$ by following a path of single-spin flips, and at each hopping the flipped variable is whitened. During this transition process, no variables of set A is flipped or whitened, as they are frozen variables. After $\vec{\sigma}^1$ is reached, as it can be completely whitened, the remaining variables (including those in set A) can all be whitened starting from the partially whitened pattern. Therefore $\vec{\sigma}^2$ can also be completely whitened and set A should be empty.

We denote the number of nonwhite variables in the solution $\vec{\sigma}^*$ of a random 3-SAT formula as N_{nw} . If the three types of clauses mentioned in Sec. II are randomly distributed in the formula, a very simple equation can be obtained for the fraction of nonwhite variables $\rho_{nw} \equiv N_{nw}/N$. Consider a randomly chosen variable node i . This node in its spin state σ_i^* is satisfying some clauses, among which n_i clauses are satisfied only by node i . The total number of clauses in the 3-SAT formula which are being satisfied by only one variable of the configuration $\vec{\sigma}^*$ is equal to zN , with z being expressed as

$$z = 3q_2\alpha, \quad (4)$$

where q_2 was defined in Sec. II. Therefore, for a large formula with $N \gg 1$, the integer n_i is distributed according to the Poisson distribution $\mathbb{P}(n_i) = e^{-z} z^{n_i} / n_i!$. The variable node i will be nonwhite if, among these n_i neighboring clauses, there is at least one clause a whose other two connected variable nodes are both nonwhite. Then the probability of a

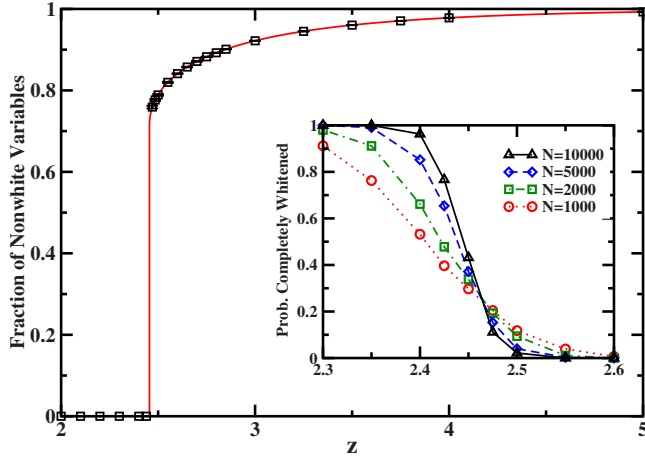


FIG. 2. (Color online) The fraction of nonwhite variables in a satisfying solution as a function of the parameter z as defined in Eq. (4). The solid line is the mean-field prediction, Eq. (5), while the square symbols are the results obtained by averaging over 50 type-B random 3-SAT formulas of size $N=10^6$. (Inset) The probability that a satisfiable solution can be completely whitened. The data points are obtained by averaging over more than 1200 randomly generated type-B 3-SAT formulas.

randomly chosen variable node i being nonwhite is determined by the following self-consistent equation:

$$\rho_{nw} = 1 - \sum_{n_i=0}^{\infty} \frac{e^{-z} z^{n_i}}{n_i!} (1 - \rho_{nw}^2)^{n_i} = 1 - \exp(-z \rho_{nw}^2). \quad (5)$$

For z less than a critical value $z_{nw}=2.45541$, Eq. (5) has only the trivial solution $\rho_{nw}=0$. While for $z > z_{nw}$, another stable positive solution of Eq. (5) appears, with $\rho_{nw} \geq 0.715332$. The freezing transition at $z=2.45541$ is a first-order bootstrap transition.

Equation (5) is confirmed to be valid for planted solutions of type-B random 3-SAT formulas (see Fig. 2). The inset of Fig. 2 shows that, when the parameter z defined in Eq. (4) increases slightly around 2.46, the probability that the planted solution of a random type-B formula can be completely whitened drops quickly from ≈ 1 to ≈ 0 , and the slope of this decrease becomes sharper for larger formulas. The values of the fraction of nonwhite variables as obtained from these simulations are in very good agreement with the mean-field prediction, Eq. (5). This good agreement indicates that the freezing phenomenon in the planted solutions of random type-B formulas can be completely explained by the formation of frozen cores.

For type-A formulas it is an empirical fact that solutions that can be found efficiently on large instances using algorithms known today are always white [18,37,38] (but see more recent simulation results of Ref. [39]). We have generated type-A random 3-SAT formulas with $N=10^6$ and constraint density $\alpha \in [4.20, 4.25]$ and used the SP algorithm to find solutions to these instances. For $\alpha=4.2$ we used in addition WALKSAT with noise parameter 0.57 since this (and other) stochastic local search heuristics are also known to be effective at these constraint densities [18,19]. Interestingly,

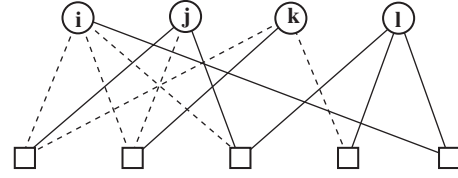


FIG. 3. Frustration effect in a completely white solution $\{\sigma_i=1, \sigma_j=1, \sigma_k=1, \sigma_l=1\}$ for a 3-SAT of $N=4$ variables and $M=5$ constraints. The variable l is frozen to the spin value $\sigma_l=1$.

the fractions of constraints satisfied by one, two, or three variables appear to depend only weakly on the constraint density and are for the solutions found by SP, $q_0 \approx 0.128$, $q_1 \approx 0.135$, and $q_2 \approx 0.157$ for all solutions of instances in this range. The solutions found by WALKSAT at $\alpha=4.2$ display also practically the same values—e.g., $q_2 \approx 0.155$. These solutions of $N=10^6$ all have a value of $z \approx 2.0$ considerably lower than the critical value z_{nw} , and all these solutions are found to be completely white. For a type-A random graph of smaller sizes $N=10^3-10^4$ and constraint density $\alpha=4.2$, besides finding many completely white solutions, the WALKSAT algorithm is also able to reach partially frozen solutions that contain a large fraction of frozen variables if a nonoptimal value of the noise parameter (e.g., $p=0.45$) is used and a long search time is permitted [43]. These non-completely white solutions also have a value of $z \approx 2.0$. The mean-field formula, Eq. (5), which does not consider any correlations in the distributions of the three types of constraints of the studied 3-SAT formula, therefore fail to describe these partially frozen solutions.

Formation of frozen cores is not the only cause of variable freezing in the solution clusters of a K -SAT formula. Figure 3 is a very simple example showing that, even if a solution to a K -SAT formula can be completely whitened, it can contain frozen variables. In the solution $\sigma_i=\sigma_j=\sigma_k=\sigma_l=1$, variable l in satisfying three white clauses. The two neighbors (i and k) of variable l are both unfrozen variables. If l is flipped to $\sigma_l=-1$, variable i should keep $\sigma_i=1$, while variable k should be flipped to $\sigma_k=-1$. Variable i then requires variable j to keep the value $\sigma_j=1$, but variable k requires j to be flipped to $\sigma_j=-1$. Such a frustration therefore prohibited variable l from taking the value $\sigma_l=-1$, although it can be whitened in the whitening process. To speak more generally, with respect to a solution $\vec{\sigma}^*$ to a K -SAT formula, let us denote by $\partial_{\sigma_i^*} i$ the set of nearest-neighboring clauses of i which are satisfied by the spin value $\sigma_i=\sigma_i^*$, and let us assume that each of these clause $a \in \partial_{\sigma_i^*} i$ can be satisfied in some solutions of the cluster associated with $\vec{\sigma}^*$ even if $\sigma_i=-\sigma_i^*$, provided that all other clauses $b \in \partial_{\sigma_i^*} a$ are removed from the formula. Then each clause in the set $\partial_{\sigma_i^*} i$ for sure can be whitened in the solution cluster. But variable i will still be frozen to the value σ_i^* if not all of these clauses can be simultaneously satisfied without the need of variable i . The second mechanism of variable freezing is therefore the closure of frustration loops. In a large random K -SAT formula, because of the existence of extremely many loops and because most of these loops are of length $\ln(N)$ or longer, this freezing mechanism is referred to as “freezing by long-range frustrations.”

Long-range frustrations were analyzed in previous studies [30,31] on ensembles of random networks. For single solutions of a given random K -SAT formula, finding all the variables which are frozen by long-range frustrations, however, is not a trivial task. In contrast to freezing by frozen-core formation, we are not yet able to construct a polynomial algorithm to identify all the long-rangely frustrated and frozen variables for a solution of a given K -SAT formula. We leave this challenge to future studies and here present instead two simple stochastic heuristic algorithms.

The first heuristic search algorithm (method 1), SPINFLIP, performs a (slightly biased) random walk in the solution cluster of the formula. Starting from a solution $\vec{\sigma}^*$ to a K -SAT formula F , SPINFLIP records and updates the current satisfying configuration of the formula and three variable sets: set V_1 contains all the variables that have already been flipped at least once (unfrozen variables), set V_2 contains all the variables that have not yet been flipped and that are currently being flippable, and set V_3 contains all the variables that belong to set V_1 and that are currently being flippable. In each elementary trial of the program, if V_2 is not empty, a variable in set V_2 is randomly chosen; otherwise a variable in set V_3 is randomly chosen; the spin of this variable is flipped, and the sets V_1 , V_2 , and V_3 are then updated. The SPINFLIP program is iterated for many steps (each of which consisting of N consecutive elementary trials) until no new unfrozen variables can be identified in the last n (say, $n=10^6$) consecutive steps. As SPINFLIP is an incomplete algorithm, it may fail to identify some unfrozen variables of a solution (that can be completely whitened), but we anticipate that most of the unfrozen variables will be discovered if the program is running for a very long time.

Besides reporting a set of unfrozen variables, the SPINFLIP program can also be used to explore the fine structure of a solution cluster [44]. The drawback of this random-walk algorithm is its slow rate of discovering new unfrozen variables. The second heuristic search algorithm (method 2) we used in this work is much faster. This later algorithm uses information obtained by the whitening program (i.e., “to flip variable i you probably should first flip variables j, k, \dots ”). At each repeat, the algorithm randomly selects a not-yet-flipped variable and propose a flip. This may cause some of the neighboring clauses (say, a) of variable i to be violated. If such a violation happens, then flip a neighboring variable j of clause a , with j being selected according to the causality relationships built by the whitening program (there are still some freedom in choosing j). This flipping process at each branch stops after a variable, which in its original spin value satisfies all its neighboring clauses, has been flipped. After the whole iteration process stops, if no clause is violated, then the proposed spin flip of variable i is accepted and all the flipped variables during this process are added to the set of unfrozen variables. As a comparison of this program (method 2) to the SPINFLIP program (method 1), we notice that, for the example shown in Fig. 5, below, SPINFLIP identifies a total number of 265 650 unfrozen variables out of 10^6 variables after running for 10^6 steps on a PC (taking about 7 weeks), while the whitening-inspired program is able to identify 265 650 unfrozen variables in a little bit less than 3 weeks. A total number of 228 167 variables appears in both

sets of unfrozen variables. If these two programs are let to run even longer, more unfrozen variables will be identified, but the rate of finding new unfrozen variables becomes very low.

IV. ENTROPIC BELIEF-PROPAGATION ALGORITHM

For a given solution $\vec{\sigma}^*$ of a satisfiable 3-SAT formula, the algorithms mentioned in the preceding section identify the set of frozen variables in the solution cluster of $\vec{\sigma}^*$. However, these algorithms do not give information about the spin value preference of each unfrozen variable node; nor do they estimate the size of the solution cluster. Now we study in more detail the statistical property of the solution cluster associated with $\vec{\sigma}^*$ by the cavity method of statistical physics [27].

According to the current statical physics picture, the satisfying solutions of a random 3-SAT formula with constraint density $\alpha > 3.86$ are distributed into exponentially many clusters, each of which in turn contains an exponential number of solutions. Different solution clusters may have different statistical properties. To characterize such a complex solution space structure, a cavity approach which corresponds to the mean-field first-step replica-symmetry-breaking spin-glass theory [27] was used in Refs. [12–14]. In the present paper, as we are interested in single-solution clusters of a random 3-SAT formula, a replica-symmetric cavity approach is exploited. This cavity approach can be expressed in terms of a set of BP iterative equations (see, e.g., Refs. [13,14,29,32]).

Before we write down the BP equations, let us notice, however, that the concept of cluster used in this section is not strictly equivalent to that defined in the preceding section III. In the mean-field spin-glass theory, a cluster (also called a macroscopic state) refers to a subspace in the system’s configuration space which satisfies the so-called clustering property [27]—namely, that the spin values of two distantly separated variable nodes are not correlated. In a macroscopic state, the point-to-set correlation between a randomly chosen variable i and variables separated from i by a shortest-path distance d also decays exponentially with this distance for d large enough (see Refs. [12,25] for more details). When this clustering property holds, in a given cluster C , the joint distribution $P(\sigma_i, \sigma_j, \dots)$ of spins for a set of distantly separated variables (i, j, \dots) can be written in a factorized form:

$$P(\sigma_i, \sigma_j, \dots) = P_i(\sigma_i)P_j(\sigma_j) \dots \quad (i, j, \dots \text{ being far apart}), \quad (6)$$

where $P_i(\sigma_i)$ is the marginal distribution of spin σ_i in cluster C . Equation (6) may not necessarily be a good approximation for a solution cluster of a satisfiable 3-SAT formula. Nevertheless, it turns out that for a large random 3-SAT formula that has a very sparse factor graph representation, if the BP iterative algorithms converge to a fixed point, it always predicts the same set of frozen variables as the whitening algorithm does. In this case, the BP approach presumably gives an accurate and comprehensive description of the solution cluster under study.

A. Iterative equations for the entropic belief-propagation algorithm

In a solution cluster for a 3-SAT formula F , we define η_i as the log-likelihood of variable i to be in the spin-up state—i.e.,

$$\eta_i \equiv \ln \left(\frac{P_i(+1)}{P_i(-1)} \right). \quad (7)$$

We also define the cavity log-likelihood $\eta_{i \rightarrow a}$ as

$$\eta_{i \rightarrow a} = \ln \left(\frac{P_{i \rightarrow a}(+1)}{P_{i \rightarrow a}(-1)} \right), \quad (8)$$

where $P_{i \rightarrow a}(\sigma_i)$ is the probability for variable i to take the spin σ_i if it is not constrained by clause a . We denote by $\exp(u_{a \rightarrow i})$ the fraction of configurations in the solution cluster in which constraint a is being satisfied by its neighboring variables j other than variable i . Under the assumption that, in the absence of constraint a , the neighboring variable nodes of a are mutually independent of each other, we can write down the following equation for $u_{a \rightarrow i}$:

$$u_{a \rightarrow i} = \ln \left[1 - \prod_{j \in \partial a \setminus i} P_{j \rightarrow a}(-J_a^j) \right], \quad (9)$$

where, according to Eq. (8), $P_{j \rightarrow a}(-J_a^j)$ is related to $\eta_{j \rightarrow a}$ through

$$P_{j \rightarrow a}(-J_a^j) = \frac{1 + J_a^j + (1 - J_a^j)e^{\eta_{j \rightarrow a}}}{2(1 + e^{\eta_{j \rightarrow a}})}. \quad (10)$$

Similarly, if we use again the factorization assumption for the neighboring clauses of a variable node i , we get the following equation for $\eta_{i \rightarrow a}$:

$$\eta_{i \rightarrow a} = \sum_{b \in \partial i \setminus a: J_b^i = -1} u_{b \rightarrow i} - \sum_{b \in \partial i \setminus a: J_b^i = +1} u_{b \rightarrow i}. \quad (11)$$

In Eqs. (9) and (11), $\partial a \setminus i$ means the set of neighboring variables except i for clause a and so on for $\partial i \setminus a$.

Equations (9) and (11) form a set of BP iterative equations, which were used in various previous studies (see, e.g., Refs. [13,14]). As we are interested in the solution cluster associated with a pre-given solution $\vec{\sigma}^*$, we use the following initial condition for this set of BP equations. On each directed edge from a variable node i to a constraint node a , at the beginning of the BP process,

$$\eta_{i \rightarrow a} = \begin{cases} +\infty & \text{if } \sigma_i^* = +1, \\ -\infty & \text{if } \sigma_i^* = -1. \end{cases} \quad (12)$$

Starting from this initial condition, the messages $\{\eta_{i \rightarrow a}, u_{a \rightarrow i}\}$ along all the edges of the factor graph of the 3-SAT formula are updated according to Eqs. (9) and (11). We have tested a synchronous and a random sequential BP iteration scheme. In the synchronous updating scheme, in one evolution step, first all the messages $u_{a \rightarrow i}$ from clauses to variables are updated using Eq. (9) and then all the messages $\eta_{i \rightarrow a}$ from variables to clauses are updated using Eq. (11). In the random sequential updating scheme, in each evolution step, first a random order (say, i_1, i_2, \dots, i_N) is made for the N variable

nodes; and for each variable node i in this order, the messages $\eta_{i \rightarrow a}$ (with $a \in \partial i$) and then $u_{b \rightarrow j}$ (with $b \in \partial i$, $j \in \partial b \setminus i$) are updated. We have checked that in instances for which the synchronous updating scheme does not drive the messages $\{\eta_{i \rightarrow a}, u_{a \rightarrow i}\}$ to a fixed point, the sequential updating scheme also fails to do so and vice versa; while if both the synchronous and the sequential updating schemes lead to convergence of the iterative equations (9) and (11), these two schemes always reach the same fixed point. This latter observation confirms that the BP fixed points reached by the BP iterative equations are stable fixed points. In the numerical simulations, the convergence condition for the BP iteration process is set to be that the maximal distance Δ (among all directed edges $a \rightarrow i$ of the graph) between the values of $e^{u_{a \rightarrow i}}$ obtained in iteration steps t and $t+1$ be less than a pre-specified value 5×10^{-6} :

$$\Delta = \max_{(a,i)} |e^{u_{a \rightarrow i}(t+1)} - e^{u_{a \rightarrow i}(t)}| < 5 \times 10^{-6}. \quad (13)$$

After the above-mentioned iteration process has reached a fixed point, the log-likelihood η_i for each variable i as defined by Eq. (7) can be calculated by

$$\eta_i = \sum_{a \in \partial i: J_a^i = -1} u_{a \rightarrow i} - \sum_{a \in \partial i: J_a^i = +1} u_{a \rightarrow i}, \quad (14)$$

and the total entropy S of the solution cluster can be estimated by the following equation:

$$S = \sum_i \Delta S_i + \sum_a \Delta S_a - \sum_{(i,a)} \Delta S_{ia}. \quad (15)$$

In Eq. (15), ΔS_i , ΔS_a , and ΔS_{ia} are, respectively, the entropy increase due to the addition of variable node i , clause node a , and the edge (i, a) between variable i and clause a , with

$$\Delta S_i = \ln \left[\exp \left(\sum_{a \in \partial i: J_a^i = -1} u_{a \rightarrow i} \right) + \exp \left(\sum_{a \in \partial i: J_a^i = +1} u_{a \rightarrow i} \right) \right], \quad (16)$$

$$\Delta S_a = \ln \left[1 - \prod_{i \in \partial a} P_{i \rightarrow a}(-J_a^i) \right], \quad (17)$$

$$\Delta S_{ia} = \ln [1 - (1 - e^{u_{a \rightarrow i}}) P_{i \rightarrow a}(-J_a^i)]. \quad (18)$$

Following the work of Chertkov and Chernyak [40], it can be shown that the entropy expression (15) corresponds to the zeroth-order term of a loop series for the entropy of the 3-SAT formula. For the sparse factor graph of a large random 3-SAT formula which contains no short loops, higher-order terms in this loop expansion should not contribute extensively to the total energy of a solution cluster, and therefore the entropy density $s \equiv S/N$ as obtained by Eq. (15) will be exact in the thermodynamic limit of $N \rightarrow \infty$.

B. Planted solutions as initial conditions for the BP algorithm

A set of type-B random 3-SAT formulas of size $N=10^6$ and different constraint densities $\alpha \geq 4.0$ are constructed, each containing a planted satisfying solution $\vec{\sigma}^*$ (see Sec. II for details). For each of these problem instances, we run the

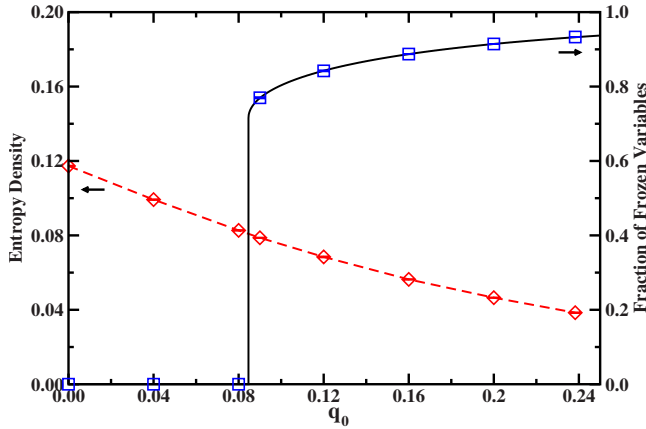


FIG. 4. (Color online) Average entropy density (diamond symbols, dashed line being a guide to the eye) and fraction of frozen variables (square symbols) for 50 randomly generated type-B 3-SAT formulas of $N=10^6$ and $\alpha=4.2$. The parameters (q_0, q_1, q_2) satisfy Eq. (19). The solid line is the fraction of nonwhite variables as predicted by Eq. (5).

BP algorithm as described above and find that it always reaches a fixed point starting from the initial condition (12). Furthermore, the set of frozen variables (i.e., variables with $\eta_i = +\infty$ or $\eta_i = -\infty$ at the fixed point) as predicted by the BP algorithm are always identical to the set of nonwhite variables discovered by the whitening algorithm of Sec. III. The convergence of the BP algorithm and the agreement with the whitening algorithm suggest that the above-mentioned replica-symmetric mean-field cavity theory is valid and that the planted solution $\vec{\sigma}^*$ can serve as an appropriate initial condition for the BP algorithm.

Figure 4 shows the BP simulation results for a set of type-B random satisfiable 3-SAT formulas which have $N=10^6$, $\alpha=4.2$, and on average equal numbers of initial satisfying and nonsatisfying edges. The later restriction is satisfied by requiring [33]

$$q_1 = (1 - 4q_0)/6, \quad q_2 = (1 + 2q_0)/6, \quad (19)$$

where q_0 , q_1 , and q_2 are defined in Sec. II. In this subensemble, the parameter q_0 (the fraction of constraints which are satisfied by three variables in configuration $\vec{\sigma}^*$) is restricted to $0 \leq q_0 \leq 0.25$. From Fig. 4 we know that as q_0 increases, the entropy density S/N of the solution cluster continuously decreases. For $q_0 \leq 0.08$, there are no frozen variables in the system (which is consistent with the prediction of Sec. III), while for $q_0 \geq 0.09$, a majority of the variables are frozen and the fraction of frozen variables is in agreement with the mean-field prediction, Eq. (5). It is interesting to note that at the freezing transition point of $q_0 \approx 0.085$, the entropy density of the system as a function of q_0 does not show any sign of singularity, while the fraction of frozen variables has a large jump. According to the mean-field cavity theory, the entropy densities of solution clusters in a completely random 3-SAT formula of $\alpha=4.2$ range from ≈ 0.060 to ≈ 0.088 [14], which are within the range of values shown in Fig. 4.

We have applied the whitening-inspired search program (method 2; see Sec. III) to the planted solutions of several type-B 3-SAT formulas. In each of these tests, this search program confirms that all the white variables of the solution are nonfrozen variables. In the cluster of a planted solution, it appears not to be any long-range frustrations. This is consistent with the fact that BP always converges with planted solutions.

V. ENTROPY OF THE CLUSTERS REACHED BY SURVEY-PROPAGATION AND WALKSAT ALGORITHMS

We also generate a set of type-A random 3-SAT formulas of size $N=10^6$ and $\alpha \in [4.20, 4.25]$ and, for each of them, use the survey-propagation algorithm to find a set of satisfying solutions. For $\alpha=4.20$ we use in addition WALKSAT as described in Sec. II. For $\alpha=3.90$ and 3.925 with $N=10^5$, solutions are also obtained by the belief-propagation-inspired decimation algorithm [12,20]. The BP algorithm is then applied in these instances, using these solutions $\vec{\sigma}^*$ as initial conditions. We find that for each problem instance, both the synchronous and sequential BP schemes predict that there are no frozen variables in the system, consistent with the result of the whitening algorithm. However, in contrast to the preceding subsection, *none* of these BP simulations converges to a fixed point of messages $\{\eta_{i \rightarrow a}, u_{a \rightarrow i}\}$. The messages $\{\eta_{i \rightarrow a}, u_{a \rightarrow i}\}$ along many edges keep fluctuating considerably around certain mean values. Different variables have different amplitudes of η and u fluctuations. In the random sequential [replica symmetric (RS)] updating scheme, these fluctuations do not show periodic patterns.

If the non-fixed-point messages $\{\eta_{i \rightarrow a}, u_{a \rightarrow i}\}$ are used to calculate the entropy, Eq. (15) reports an entropy density value of $s \approx 0.090$ at $\alpha=4.2$, which is equal to the replica-symmetric entropy density as calculated in earlier studies [see Fig. 2 of Ref. [14] or [13]]. We have further checked that, if the BP iteration starts from the RS initial condition $\{\eta_{i \rightarrow a} = 0\}$, the evolution trajectory of the messages $(\eta_{j \rightarrow b}, u_{b \rightarrow j})$ on any given edge (j, b) cannot be distinguished from the evolution trajectories starting from a SP or WALKSAT solution. The BP algorithm therefore in some sense forgets its starting point and does not bring us any cluster-specific information.

The nonconvergence of BP is not due to the different 3-SAT ensemble used in this section, but is related with the initial conditions used in the BP. To support this claim, we notice that for the type-B random formulas with $q_0 > 0.01$ studied in Fig. 4 of the preceding section, when SP or WALKSAT solutions instead of planted solutions are used as initial conditions for the BP algorithm, the BP algorithm fails to converge. At $\alpha=4.2$ and $q_0 > 0.01$, solutions found by the SP or WALKSAT algorithm are not in the same cluster as the planted solution. The planted solution correspond to a “crystal” phase, while the SP and WALKSAT solutions all belong to the “glassy” phase. The set of type-B random formulas with $q_0 < 0.01$ used in Fig. 4 are in the replica-symmetric phase (only one solution cluster), and then the BP algorithm converges to the same fixed point independent of initial conditions.

As we mentioned in Sec. III, variable freezing can be caused by long-range frustrations [30,31]. As an example, the SPINFLIP algorithm was only able to confirm that 25% of the variables are unfrozen in a completely white SP solution for a type-A 3-SAT formula with $N=10^6$ variables and constraint density $\alpha=4.25$, even after running for 7 weeks. (The whitening-inspired search algorithm performs a little bit better; it reported that 26.5% of the variables in the same solution are unfrozen, after running for about 3 weeks.) As the BP algorithm uses only local structural information of a graph, it is unable to detect the globally constrained variables. Some of the variables in the solution can be externally fixed to make BP converge. For this exemplar solution, in Fig. 5(a) we plot the number of newly whitened variables at each step of the whitening process and show how many of them are also identified as unfrozen variables by the two heuristic programs. At earlier steps ($t \leq 25$) of the whitening process, most of the whitened variables are confirmed to be unfrozen variables, but at later whitening steps most of the newly whitened variables are very difficult to be flipped (if not impossible). This is expected: as long-range frustration effects are strongly related to the closure of loops in the graph, only variables which are whitened at steps of order $\ln(N)$ (the typical length of a loop) or later can have a large probability of being frozen or extremely constrained. Since variables that are whitened in the later steps of the whitening process are extremely difficult to be flipped, they must be extremely constrained in the reference solution $\vec{\sigma}^*$. Figure 5(a) then suggests that a way to make BP converge is to externally fix the spin values of variables which are newly whitened in certain whitening step (say, t). If these variables are fixed, the whitening program can not proceed to the next step $t+1$, and the BP algorithm, which is capable of detecting frozen cores, will then predict all variables corresponding to steps $\geq t+1$ in Fig. 5(a) to be frozen.

Figure 5(b) shows the results of the BP algorithm after externally fixing a group of variables. When the spin values of the variables corresponding to whitening step t are all externally fixed, the BP iteration converges to a fixed point as long as $t \leq 32$. The calculated entropy density value increases with t only very slowly, and the predicted number of frozen variables decreases with t . The BP algorithm fails to converge when the externally fixed variables are from whitening step $t \geq 33$ [the parameter Δ as defined in Eq. (13) is about 0.5 even after 2×10^4 iteration steps]. Therefore we take the value of $s=0.0641$ obtained at $t=32$ as the entropy density of the solution cluster. The fraction of frozen variables is predicted to be 0.7472 at $t=32$, while from the result of the two heuristic search programs [see Fig. 5(a)] we know that the real fraction of frozen variables should be at most 0.713. It appears that more variables should be in the frozen state for BP to converge: if we run the BP iteration by externally fixing all the frozen variables reported by either of the two search programs, the BP algorithm again fails to converge. It is tempting for us to interpret this observation as follows: The solution cluster can be divided into many subclusters; in each subcluster, besides those variables that are frozen in all subclusters, some additional variables are frozen. For a very large random K -SAT formula, as there are exponentially many different combinatorial ways to choose

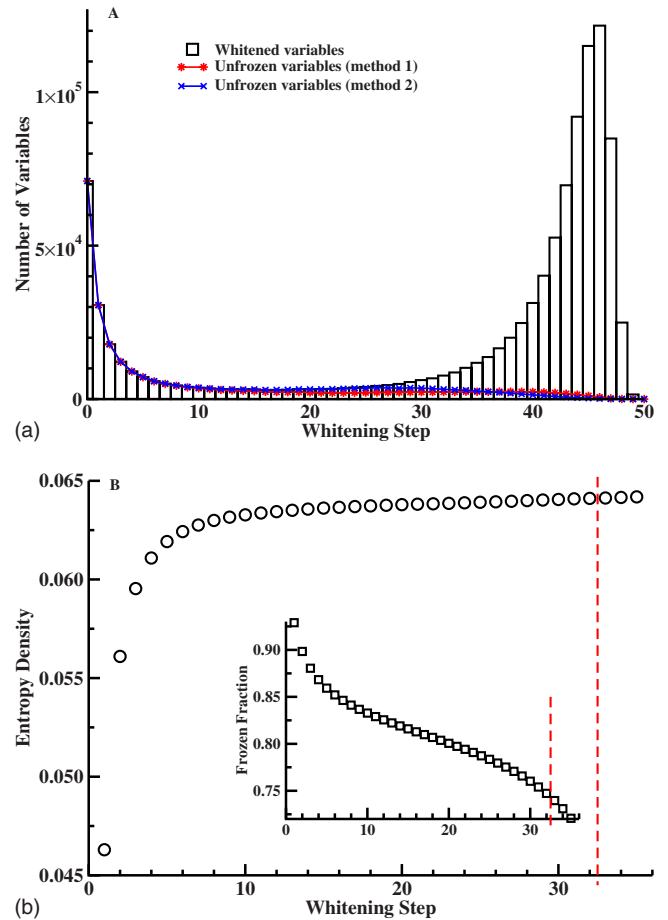


FIG. 5. (Color online) (a) The $N=10^6$ variables of a random type-A 3-SAT formula with $M=4.25 \times 10^6$ constraints is grouped into 51 sets according to which step t they are whitened by the whitening algorithm. The SPINFLIP algorithm (method 1) identified 249 923 variables to be unfrozen after making $10^6 \times N$ spin flips (in about 7 weeks), while the whitening-inspired algorithm (method 2) identified 265 650 variables to be unfrozen after running for about 3 weeks. The distribution of these unfrozen variables in each group is shown. The reference solution is obtained by the SP algorithm. (b) The entropy density and fraction of frozen variables as predicted by the BP algorithm when the spin values of all the variables whitened at step t of the whitening process are being externally fixed. The BP algorithm becomes nonconvergent at $t \geq 33$ (marked by the dashed lines).

these additional subcluster-specific frozen variables, probably the number of subclusters is also exponential. These subclusters are not separated with each other by any energy barriers; they are formed by correlation properties. This conjectured further structural organization in a single-solution cluster will be checked by a future investigation.

We have applied this combined BP and whitening approach to a set of other type-A random 3-SAT formulas and SP and WALKSAT solutions. Some of the results are reported in Fig. 6. At $\alpha=4.20$, the entropy densities of the solution clusters reached by SP and WALKSAT are comparable, being $s \approx 0.0725$ and $s \approx 0.0715$, respectively. In comparison, the dominant clusters of the random 3-SAT problem has entropy density $s \approx 0.088$ and the most abundant clusters have en-

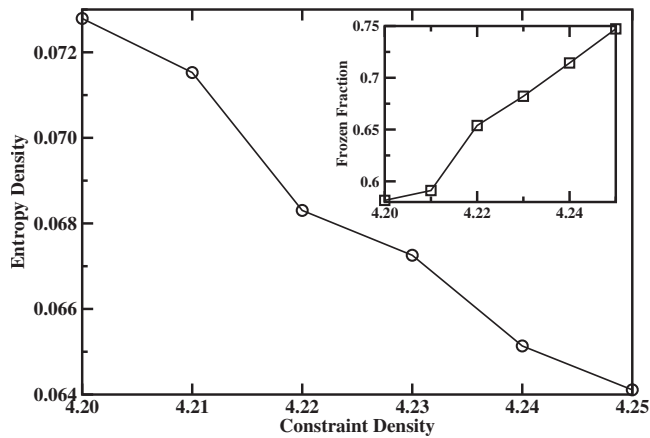


FIG. 6. The entropy density of a SP solution-associated solution cluster for a random 3-SAT formula of size $N=10^6$. The fraction of frozen variables in the solution cluster as predicted by BP is also shown. Each data point is obtained by running BP on a single SP solution by externally fixing a tiny fraction of variables.

entropy density $s \approx 0.060$ [14]. At $\alpha=4.25$, the clusters reached by SP have entropy density $s \approx 0.064$, while the dominating and most abundant clusters have entropy density values $s \approx 0.068$ and $s \approx 0.060$, respectively [14]. It appears that solutions reached by SP and WALKSAT belong neither to one of the dominating clusters nor to one of the most abundant clusters (the same observation was obtained in Ref. [41] for the random bicoloring problem).

We close this section by mentioning that another way of making the BP algorithm converge to a fixed point is by damping [42]. This strategy was not used in the present work because we were not yet very clear of the physical meaning of the converged fixed point of the damped BP algorithm [42]. As explained in this section, the action of externally fixing some variables to make the BP algorithm converge is physically reasonable, as most of the predicted frozen variables by the resulting BP fixed point are highly constrained variables and very difficult to be flipped [see Fig. 5(a)]. Explicitly fixing these variables helps to remove possible long-range correlations within the solution cluster of the 3-SAT formula. Figure 5(b) demonstrates that the calculated entropy value is not sensitive to the set of variables that are being externally fixed. Another different strategy was used in Ref. [41] to calculate the entropy of a single-solution cluster.

VI. CONCLUSION

In this paper we have studied the statistical property of solution clusters that are associated with single solutions of a random 3-SAT formula. It was pointed out that there are two different mechanisms for the freezing of variables in a solution cluster. Variables that are frozen due to frozen-core formation can easily be identified by both the whitening and the belief-propagation algorithm. But variables that are frozen due to long-range frustrations can be very difficult to be identified, as long-range frustrations involve global and topological properties of the 3-SAT formula. A heuristic search algorithm, SPINFLIP, was constructed to search for such variables.

When long-range frustrations exist in a solution $\vec{\sigma}^*$ and the associated cluster of random 3-SAT formula, the BP iteration process starting from the initial condition $\vec{\sigma}^*$ is unable to reach a fixed point. To overcome this difficulty, a tiny set of variables (chosen with the help of the whitening algorithm) was externally fixed to their initial spin values during the BP iteration. When this modified BP process reaches a fixed point, the entropy densities of the solution cluster were evaluated. It was found that at $4.2 \leq \alpha \leq 4.25$, the solutions obtained by SP or WALKSAT for a given random 3-SAT problem are in medium-sized clusters; their entropy densities are higher than the entropy density of the most abundant clusters in the formula, but lower than the entropy density of the most dominating clusters.

The present work indicates that at constraint density α close to the satisfiability threshold, a single-solution cluster of a random 3-SAT formula can be further divided into sub-clusters. Such further structural organizations, if they exist, may be described using the first-step replica-symmetry-breaking (RSB) spin-glass cavity theory [8,27]. Further work along this line will be reported in another paper.

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