Witness of unsatisfiability for a random 3-satisfiability formula

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The random 3-satisfiability (3-SAT) problem is in the unsatisfiable (UNSAT) phase when the clause density α exceeds a critical value $\alpha_s \approx 4.267$. Rigorously proving the unsatisfiability of a given large 3-SAT instance is, however, extremely difficult. In this paper we apply the mean-field theory of statistical physics to the unsatisfiability problem, and show that a reduction to 3-XORSAT, which permits the construction of a specific type of UNSAT witnesses (Feige-Kim-Ofek witnesses), is possible when the clause density $\alpha > 19$. We then construct Feige-Kim-Ofek witnesses for single 3-SAT instances through a simple random sampling algorithm and a focused local search algorithm. The random sampling algorithm works only when α scales at least linearly with the variable number N, but the focused local search algorithm works for clause density $\alpha > cN^b$ with $b \approx 0.59$ and prefactor $c \approx 8$. The exponent b can be further decreased by enlarging the single parameter S of the focused local search algorithm.

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I. INTRODUCTION

The satisfiability (SAT) problem is a constraint satisfaction problem of great practical and theoretical importance. On the practical side, many constraint satisfaction problems and combinatorial optimization problems in industry and engineering can be converted into a SAT problem; therefore many heuristic solution-searching algorithms have been developed over the years for single problem instances (see review [1]). On the theoretical side, the SAT problem is the first constraint satisfaction problem shown to be non-deterministic polynomial (NP) complete [2,3]; all other NP-complete problems can be transformed into the SAT problem through a polynomial number of steps. Understanding the computational complexity of the SAT problem has attracted a lot of research efforts.

The ensemble of random K-SAT problems has been the focus of intensive theoretical studies by computer scientists and statistical physicists in the last 20 years [4–11]. In a given instance (formula) of the random K-SAT problem, the states of N binary variables are constrained by M clauses, with each clause involving a fixed number K of variables, randomly and independently chosen from the whole set of N variables. The clause density is defined as

$$\alpha \equiv \frac{M}{N},$$

which is just the ratio between the clause number M and the variable number N.

The random K-SAT problem has a critical clause density $\alpha_s(K)$ at which a satisfiability transition occurs. At the thermodynamic limit of $N \to \infty$, all the M clauses of an instance of the random K-SAT problem can be simultaneously satisfied if the clause density $\alpha < \alpha_s(K)$, but this becomes impossible if $\alpha > \alpha_s(K)$. The value of $\alpha_s(K)$ for $K \geqslant 3$ can be estimated by the mean-field theory of statistical physics [8,9,12]. For example, $\alpha_s(3) = 4.267$ for the random 3-SAT problem.

Most previous investigations on the random K-SAT problem considered the SAT phase, $\alpha < \alpha_s(K)$. To prove a K-SAT formula is satisfiable, it is sufficient to show that there exists a single spin configuration of the N variables which makes all the M clauses to be simultaneously satisfied. However, to certify a K-SAT formula to be unsatisfiable is much harder. In principle, one has to show that none of the 2^N spin configurations satisfies the M clauses simultaneously.

Theoretical computer scientists have approached the K-SAT problem from the UNSAT phase through spectral algorithms [13–15]. These refutation algorithms are able to certify the unsatisfiability of random 3-SAT formulas when $\alpha > cN^{\frac{1}{2}}$ (where the constant c should be sufficiently large). The refutation lower bound for random 3-SAT was further pushed to $\alpha > cN^{\frac{2}{5}}$ by Feige *et al.* [16] from another theoretical approach, namely, treating a given 3-SAT instance also as a 3-exclusive or (3-XORSAT) instance. Feige and coauthors [16] observed that if a 3-SAT formula is satisfiable, the global minimum number of unsatisfied clauses of the formula treated as a 3-XORSAT cannot exceed a certain value. Proving the unsatisfiability of a 3-SAT instance is thus converted to constructing a high-enough lower bound for the ground-state energy (i.e., the global minimum number

of unsatisfied clauses) of the corresponding 3-XORSAT formula.

Using 3-XORSAT to prove a result on 3-SAT is in computer science terminology a *reduction*, while a specific high-enough lower bound is a *witness of unsatisfiability*. In this paper we study two related questions. The first is if the reduction is possible in random 3-SAT formulas with large but constant clause density α. Using the (nonrigorous) mean-field method of statistical physics, we answer this question affirmatively, provided clause density $\alpha > 19$. This means that when $\alpha < 19$ the ground-state energy of a random 3-XORSAT instance is (almost surely, in the thermodynamic limit) lower than the value which would allow us to conclude that the corresponding 3-SAT instance is unsatisfiable. If, on the other hand, $\alpha > 19$, then the ground-state energy of a random 3-XORSAT instance is (almost surely, in the thermodynamic limit) high enough, and it should in principle be possible to find witnesses of unsatisfiability. The method of Ref. [16] also gives, apart from the reduction of 3-SAT to 3-XORSAT, a constructive procedure to construct the lower bound. In this paper we refer to such witnesses as Feige-Kim-Ofek (FKO) [16] witnesses.

The second issue addressed in this paper is then to construct FKO witnesses, which is expected to be very difficult for such sparse formulas. A very simple random sampling algorithm is tested in this paper. Without any optimization, the performance of this naive algorithm is not good; it only works for α scaling at least linearly with N. We then test the performance of a simple focused local search algorithm. We find this algorithm performs much better. It can construct UNSAT witnesses for 3-SAT instances with clause density $\alpha > 8N^{0.59}$. Further improvements are observed when some modifications are made on this focused local search algorithm.

The paper is structured as follows: In Sec. II we review the main ideas behind the reduction and FKO witnesses; Sec. III demonstrates the reduction for the sparse random 3-SAT problem; and Sec. IV shows the performances of the naive random sampling algorithm and the focused local search algorithm. In Sect. V we conclude and discuss further directions of this work.

II. THE FEIGE-KIM-OFEK WITNESS

Consider a system with N variables $i \in \{1,2,\ldots,N\}$. Each variable i has a (binary) spin state $\sigma_i \in \{-1,+1\}$. A configuration of the system is denoted as $\underline{\sigma} \equiv (\sigma_1,\sigma_2,\ldots,\sigma_N)$, and there are a total number 2^N of such configurations. The system has also M clauses $a \in \{1,2,\ldots,M\}$. Each clause a is a constraint over $K = 3$ different variables (say i,j,k) and it has three coupling constants (say J_a^i, J_a^j, J_a^k), each of which is either $+1$ or -1. We consider two types of energies for clause a, namely, the SAT energy

$$E_a^{\rm sat}(\sigma_i,\sigma_j,\sigma_k) = \frac{\left(1 - J_a^i\sigma_i\right)\left(1 - J_a^j\sigma_j\right)\left(1 - J_a^k\sigma_k\right)}{8} \qquad (1)$$

and the XORSAT energy

$$E_a^{\rm xor}(\sigma_i,\sigma_j,\sigma_k) = \frac{1 - J_a^i J_a^j J_a^k \sigma_i\sigma_j\sigma_k}{2}. \qquad (2)$$

If the total energy of the system is defined as the sum of all the SAT energies, then the problem is a 3-SAT formula with energy function

$$E^{\rm sat}(\underline{\sigma}) = \sum_{a=1}^{M} E_a^{\rm sat}. \qquad (3)$$

A configuration $\underline{\sigma}$ is referred to as a satisfying assignment (or a solution) for the 3-SAT formula if its energy $E^{\rm sat}(\underline{\sigma}) = 0$. The 3-SAT formula is referred to as satisfiable (SAT) if there exists at least one satisfying assignment for this formula; otherwise it is referred to as unsatisfiable (UNSAT).

For the same set of M clauses, we can also consider all the XORSAT energies and define a 3-XORSAT formula with energy function

$$E^{\rm xor}(\underline{\sigma}) = \sum_{a=1}^{M} E_a^{\rm xor}. \qquad (4)$$

The ground-state (i.e., global minimum) energy of the XOR-SAT energy is denoted as $E_0^{\rm xor}$:

$$E_0^{\rm xor} \equiv \min_{\underline{\sigma}} E^{\rm xor}(\underline{\sigma}).$$

Checking whether a 3-XORSAT formula is satisfiable (namely, $E_0^{\rm xor} = 0$) is an easy computational task (it is a linear problem and therefore can be solved by Gaussian elimination). However, if $E_0^{\rm xor} > 0$, to determine the precise value of $E_0^{\rm xor}$ is a NP-hard computational problem (see [17] for a pedagogical explanation of this interesting issue).

The constrained system can be conveniently represented as a bipartite graph with N circular nodes for the variables, M square nodes for the constraint clauses, and $3M$ edges between the variable nodes and the clause nodes (see Fig. 1). Such a bipartite graph is often referred to as a factor graph [18]. In the factor graph, each clause a is connected by three edges to the three constrained variables, and the edge (i,a) between a variable i and a clause a is shown as a solid line (if $J_a^i = 1$) or a dashed line (if $J_a^i = -1$). In the factor graph of the system, the number of attached edges of different variables might be different. For a variable i the number of attached positive and negative edges is denoted as k_i^+ and k_i^-, respectively.

To prove the unsatisfiability of a 3-SAT formula is very challenging, since in principle one has to show that for each of the 2^N configurations, the SAT energy $E^{\rm sat}(\underline{\sigma}) > 0$, but such an enumeration becomes impossible for systems with $N > 100$. Feige, Kim, and Ofek (FKO) [16] approached this problem with the proposal of constructing UNSAT witnesses through the 3-XORSAT energy (4). Here we review their main ideas [16].

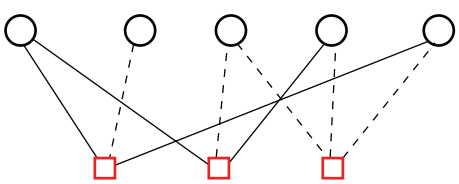

FIG. 1. (Color online) Factor graph representation for a 3-SAT formula. The variables and clauses are represented by circles and squares, respectively. Each clause has three edges attached. A solid edge between a variable i and a clause a means that the coupling constant $J_a^i = 1$, while a dashed edge means that $J_a^i = -1$.

Consider a given 3-SAT formula with energy function (3). Suppose this formula is satisfiable, then there is at least one satisfying configuration $\underline{\sigma}$ such that $E^{\rm sat}(\underline{\sigma})=0$. An edge (i,a) is referred to as being satisfied by $\underline{\sigma}$ if (and only if) the spin of variable i is $\sigma_i = J_a^i$ in this configuration. With respect to $\underline{\sigma}$, the total number of clauses containing one, two, and three satisfied edges is denoted as M_1, M_2, and M_3, respectively. These three integers satisfy the following two relations:

$$M_1 + M_2 + M_3 = M, \tag{5}$$

$$M_1 + 2M_2 + 3M_3 \leqslant \frac{3M}{2} + \frac{1}{2}\sum_{i=1}^{N} |k_i^+ - k_i^-|. \tag{6}$$

Equation (5) is a consequence of the assumption that $E^{\rm sat}(\underline{\sigma}) = 0$, while Eq. (6) is due to the fact that each variable i in its spin state σ_i can satisfy at most $\max(k_i^+,k_i^-)$ edges. The above two expressions lead to

$$M_2 \leqslant 2M_{12} - \frac{3}{2}M + \frac{1}{2}\sum_{i=1}^{N} |k_i^+ - k_i^-|, \tag{7}$$

where $M_{12} \equiv M_1 + M_2$.

On the other hand, it is very easy to check that the 3-XORSAT energy (4) of the configuration $\underline{\sigma}$ is just $E^{\rm xor}(\underline{\sigma}) = M_2$. Therefore if $E^{\rm sat}(\underline{\sigma})=0$, then the 3-XORSAT ground-state energy $E_0^{\rm xor}$ must not exceed M_2. If $E_0^{\rm xor}$ exceeds M_2, then the 3-SAT energy function (3) must be positive for all the 2^N configurations. A high-enough 3-XORSAT ground-state energy then serves as a FKO witness that the corresponding 3-SAT formula is UNSAT.

Consider any spin configuration $\underline{\sigma}$ (not necessarily a configuration with $E^{\rm sat}(\underline{\sigma})=0$). The value of M_{12} in Eq. (7) is then calculated as

$$M_{12} = \sum_{a=1}^{M} \frac{\left(3+\sum_{i\in\partial a}\sigma_i J_a^i\right)\left(3-\sum_{j\in\partial a}\sigma_j J_a^j\right)}{8} \tag{8}$$

$$= \sum_{a=1}^{M} \frac{9-\sum_i\sum_j \sigma_i\sigma_j J_a^i J_a^j}{8} \tag{9}$$

$$= \frac{1}{4}\left(3M + \sum_{i,j}\sigma_i \mathcal{M}_{ij}\sigma_j\right), \tag{10}$$

where the matrix element $\mathcal{M}_{ij}$ is defined as

$$\mathcal{M}_{ij} = \begin{cases} -\frac{1}{2}\sum_{a\in\partial i\cap\partial j} J_a^i J_a^j & \text{for } i\neq j, \\ 0 & \text{for } i=j. \end{cases} \tag{11}$$

In the above expressions, ∂a denotes the set of variables that are connected to clause a by an edge, and ∂i denotes the set of clauses that are connected to variable i by an edge, and $\partial i\cap\partial j$ denotes the intersection of ∂i and ∂j.

The maximal eigenvalue of the symmetric matrix formed by the elements $\mathcal{M}_{ij}$ is denoted as λ. This eigenvalue satisfies

$$\lambda \geqslant \frac{\sum_{i,j} y_i \mathcal{M}_{ij} y_j}{\sum_i y_i^2} \tag{12}$$

for any nonzero real vector $\underline{y} = (y_1, y_2, \ldots, y_n)$. Take $y_i = \sigma_i$ for each variable i, and it is then easy to show that $\lambda \geqslant (4M_{12} - 3M)/N$. Combining this with (7), an upper bound $M_2^{\rm upp}$ for M_2 is obtained as

$$M_2 \leqslant M_2^{\rm upp} \equiv \frac{1}{2}N\lambda + \frac{1}{2}\sum_{i=1}^{N}|k_i^+ - k_i^-|. \tag{13}$$

If $E_0^{\rm xor} > M_2^{\rm upp}$ for the given 3-SAT instance, then the instance must be unsatisfiable.

III. THE REDUCTION OF SPARSE RANDOM 3-SAT TO 3-XORSAT

Feige and coauthors [16] have studied the existence of FKO witness for random 3-SAT factor graphs. A random 3-SAT factor graph with N variables and M clauses is a random bipartite graph, with each clause being connected to three randomly chosen different variables and the edge coupling constant being assigned the value $+1$ or -1 with equal probability. In the large N limit, it was proved mathematically in [16] that, if the clause density α grows with N such that

$$\alpha > cN^{0.4} \tag{14}$$

with a sufficiently large constant c, then FKO witness exists with probability approaching 1 for a random 3-SAT factor graph of N variables and αN clauses.

However, it is not yet known whether witnesses of unsatisfiability exist also for random 3-SAT factor graphs with a large but constant clause density α. Here we demonstrate using the mean-field statistical physics method that the ground-state energy of random 3-XORSAT is (in the thermodynamic limit, $N\to\infty$) sufficiently large if $\alpha > 19$. This estimated constant lower bound of clause density is much improved as compared to Eq. (14).

According to Eq. (8), the quantity M_{12} can be expressed as

$$M_{12} = M - \sum_{a=1}^{M}\delta\left(\left|\sum_{j\in\partial a} J_a^j\sigma_j\right| - 3\right), \tag{15}$$

where $\delta(x)$ is the Kronecker symbol, with $\delta(x)=0$ if $x\neq 0$ and $\delta(x)=1$ if $x=0$. Combining Eq. (15) with Eq. (7), we obtain another upper bound for M_2 as

$$M_2^{\max} = \frac{1}{2}\left(M + \sum_{i=1}^{N}|k_i^+ - k_i^-|\right) - 2\min_{\underline{\sigma}}\left[\sum_{a=1}^{M}\delta\left(\left|\sum_{j\in\partial a} J_a^j\sigma_j\right| - 3\right)\right]. \tag{16}$$

The first term on the right of Eq. (16) is easy to calculate, while the minimum of the second term over all the configurations $\underline{\sigma}$ can be evaluated by the zero-temperature first-step replica-symmetry-breaking (1RSB) cavity method [9,19–21]. (Technical details of the computation are given in the Appendix.) The upper-bound $M_2^{\max}$ is tighter (smaller) than the upper-bound $M_2^{\rm upp}$ of Eq. (13).

The global minimum $E_0^{\rm xor}$ of the 3-XORSAT energy (4) can also be evaluated similarly using the zero-temperature 1RSB cavity method [19]. Figure 2 is the comparison between the value $M_2^{\max}/N$ and the ground-state energy density $E_0^{\rm xor}/N$ of (4) using clause density α as the control parameter.

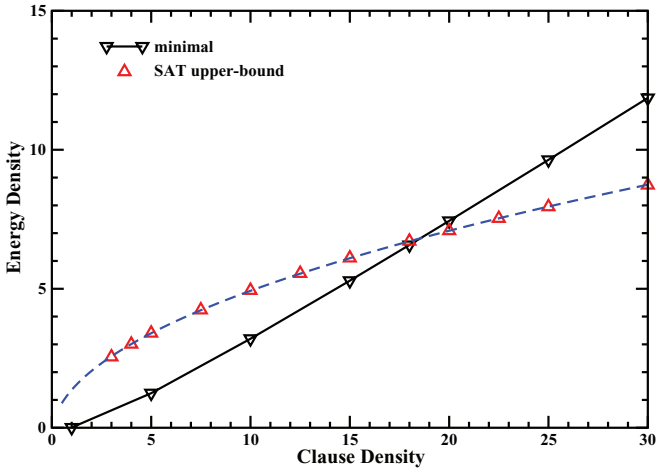

FIG. 2. (Color online) The down triangles connected by the solid line are the minimum energy density $E_0^{\rm xor}/N$ of the 3-XORSAT formula (4). The upper triangles are the upper-bound $M_2^{\rm max}/N$ obtained by Eq. (16) under the assumption that the 3-SAT energy (3) is satisfiable. The dashed line is a fitting curve of the form $M_2^{\rm max}/N = c_1 + c_2\sqrt{\alpha}$. For $\alpha > 19$ the predicted upper bound is lower than the global minimum, indicating that the assumption that Eq. (3) is satisfiable must be wrong.

When $\alpha > 19$, the requirement of ground-state energy density $E_0^{\rm xor}/N$ being lower than the upper-bound $M_2^{\rm max}/N$ is violated, which gives an indication that the 3-SAT energy function (3) has no zero-energy configurations. However, when $\alpha < 19$, $E_0^{\rm xor}/N < M_2^{\rm max}/N$ is consistent with the assumption that the 3-SAT formula is satisfiable, indicating that the reduction to 3-XORSAT cannot be used for the most difficult region of $\alpha < 19$.

Previous stability analysis [22] has suggested that the zero-temperature 1RSB mean-field theory is not completely sufficient for calculating the ground-state energy density of a finite-connectivity spin glass model. One has to extend the theory to infinite steps of replica symmetry breaking to get a marginally stable mean-field solution. However, experiences obtained on the minimal vertex cover problem [23] and other combinatorial optimization problems [21] have indicated that even though the 1RSB mean-field solution is not stable, the ground-state energy density predicted by this solution is actually very close to the true value. We therefore believe that the crossing point of the two curves of Fig. 2 will have no noticeable change, even if using a more sophisticated mean-field theory.

It is empirically well known that the random 3-SAT problem is hardest when the clause density α is close to the satisfiability threshold $\alpha_s(3) = 4.267$ [8,9,12]. Figure 2 suggests that only a finite interval up to $\alpha \approx 19$ is truly hard, with the proviso that it is not enough to know that good enough lower bounds can be found in principle; we must also find them in practice. In Sect. IV we discuss how this can be done for FKO witnesses.

IV. WITNESS CONSTRUCTION

The reduction works if we can show that the ground-state energy $E_0^{\rm xor}$ of the 3-XORSAT formula (4) is higher than either $M_2^{\rm max}$ or $M_2^{\rm upp}$. While the value of $M_2^{\rm upp}$ is easy to calculate, the exact determination of $E_0^{\rm xor}$ is a NP-hard computational problem. Feige and coauthors circumvented this computational difficulty by constructing a lower bound for $E_0^{\rm xor}$ [16]. If the value of this lower bound is higher than $M_2^{\rm upp}$, it is guaranteed that $E_0^{\rm xor} > M_2^{\rm upp}$.

A. A lower bound on $E_0^{\rm xor}$

Given a 3-SAT formula F with N variables and M clauses, a subformula f is obtained by choosing m clauses from the M clauses. For such a subformula f its 3-SAT energy and 3-XORSAT energy can be defined similar to Eqs. (3) and (4). It is computationally easy to determine whether a subformula f is 3-XORSAT satisfiable.

It was noted in Ref. [16] that for a 3-SAT formula F, if t subformulas can be constructed such that each of them is unsatisfiable as 3-XORSAT, and each clause of F appears in at most of the t subformulas d, such that

$$\frac{t}{d} > M_2^{\rm upp}, \tag{17}$$

then the formula F is unsatisfiable as 3-SAT.

To prove this statement, we simply notice that if F is satisfiable as 3-SAT, the minimum number of simultaneously unsatisfied clauses as 3-XORSAT cannot exceed $M_2^{\rm upp}$. On the other hand, there are t unsatisfiable 3-XORSAT subformulas, meaning that at least t clauses (some of them might be identical) are simultaneously unsatisfied (as 3-XORSAT) by any spin configuration. Since each clause can be present in at most d different subformulas, the total number of simultaneously unsatisfied different clauses is at least t/d [16].

Let us point out a simple improvement over the criterion Eq. (17). Suppose we have a set of t unsatisfiable 3-XORSAT subformulas constructed from the 3-SAT formula F. Let us denote by d_a the number of times clause a appears in these subformulas. Let us rank the M values of d_a in descending order and denote the ordered values as $\{d^{(1)},d^{(2)},\ldots,d^{(M)}\}$, with $d^{(1)} \geqslant d^{(2)} \geqslant \cdots \geqslant d^{(M)}$. A better refutation inequality can be written as

$$C > M_2^{\rm upp}, \tag{18}$$

where C is the minimal integer satisfying

$$\sum_{a=1}^{C} d^{(a)} \geqslant t. \tag{19}$$

To prove that (18) ensures the unsatisfiability of the 3-SAT formula F, we only need to show that the ground-state energy $E_0^{\rm xor}$ of the 3-XORSAT energy (4) cannot be lower than C. We reason as follows. To make F satisfiable as 3-XORSAT, some clauses have to be removed from F in such a way that for each of the t constructed unsatisfiable subformulas, at least one of the involved clauses should be removed. Therefore the sum of numbers d_a of the removed clauses should be at least t. This then proves the refutation inequality (18). The quantity C as obtained by Eq. (19) is a lower bound of $E_0^{\rm xor}$. This lower bound actually is not tight. It is much lower than the true ground-state energy.

B. Random sampling

A simple way of constructing an unsatisfiability witness through 3-XORSAT for a given 3-SAT formula F is the following:

(**0**) Calculate $\sum_i |k_i^+ - k_i^-|$ and the maximal eigenvalue λ of matrix $\mathcal{M}$ for formula F. Set the subformula number as $t = 0$ and set the counting number $d_a = 0$ for each clause a of F.

(**1**) Randomly select N^γ variables from the set of N variables, where $\gamma \in [0,1]$ is a fixed parameter.

(**2**) Check if the subformula f of F induced by these N^γ variables is 3-XORSAT satisfiable, and if yes, go back to step **1**. Otherwise an unsatisfiable 3-XORSAT formula is obtained.

(**3**) Construct a subformula $\tilde{f}$ by adding clauses of f one after the other in a random order, until $\tilde{f}$ becomes unsatisfiable (and has ground-state energy 1) as 3-XORSAT. Then prune the subformula $\tilde{f}$ by recursively removing those variables that are connected to only one clause and the associated single clauses. After this leaf-removal process is finished, we obtain an unsatisfiable core subformula. The counting number d_a of each clause of this core subformula is increased by one ($d_a \leftarrow d_a + 1$), and the subformula number is also increased by one ($t \leftarrow t + 1$).

(**4**) Calculate C according to (19) and then check if (18) is satisfied. If yes, output "UNSAT witness found"; otherwise, repeat steps **1**–**4**.

Figure 3 shows the simulation results on two single 3-SAT instances. The upper panel A is a 3-SAT formula with 100 variables and clause density $\alpha = 100$, and the lower panel B is another 3-SAT formula with 100 variables and clause density $\alpha = 400$. If the curve $C(t)$ is able to go beyond $M_2^{\rm upp}$ (marked by the horizontal dashed line), then a FKO witness is found. The random sampling algorithm succeeded in finding a FKO witness for the instance with $\alpha = 400$ but failed to do so for the one with $\alpha = 100$.

For $N \gg 1$, a random subformula constructed by the above-mentioned procedure contains about $0.633N^\gamma$ clauses [24]. When there are a large number t of such subformulas, the total number of clauses is about $0.633tN^\gamma$, and each clause appears on average in $\overline{d} = 0.633tN^\gamma/M$ subformulas. From this we estimate that the solution C of (19) is roughly

$$C \sim \frac{t}{\overline{d}} \approx \frac{M}{N^\gamma} = \alpha N^{1-\gamma}. \tag{20}$$

On the other hand, $M_2^{\rm upp}$ scales as $\alpha^{1/2}N$ (see Fig. 2 and [16]). Therefore we see that for the inequality (18) to hold, it is required that

$$\alpha > N^{2\gamma}. \tag{21}$$

The average number of clauses among a randomly chosen N^γ variables is about $N^{3\gamma-3}M = \alpha N^{3\gamma-2}$. This value should be proportional to N^γ so that the subformula induced by these variables has a high probability to be unsatisfiable as 3-XORSAT. Therefore we require that $\alpha N^{3\gamma-2} \approx N^\gamma$, from which we get

$$\alpha \approx N^{2-2\gamma}. \tag{22}$$

From Eqs. (21) and (22) we obtain that the parameter γ should be chosen as

$$\gamma = \tfrac{1}{2}. \tag{23}$$

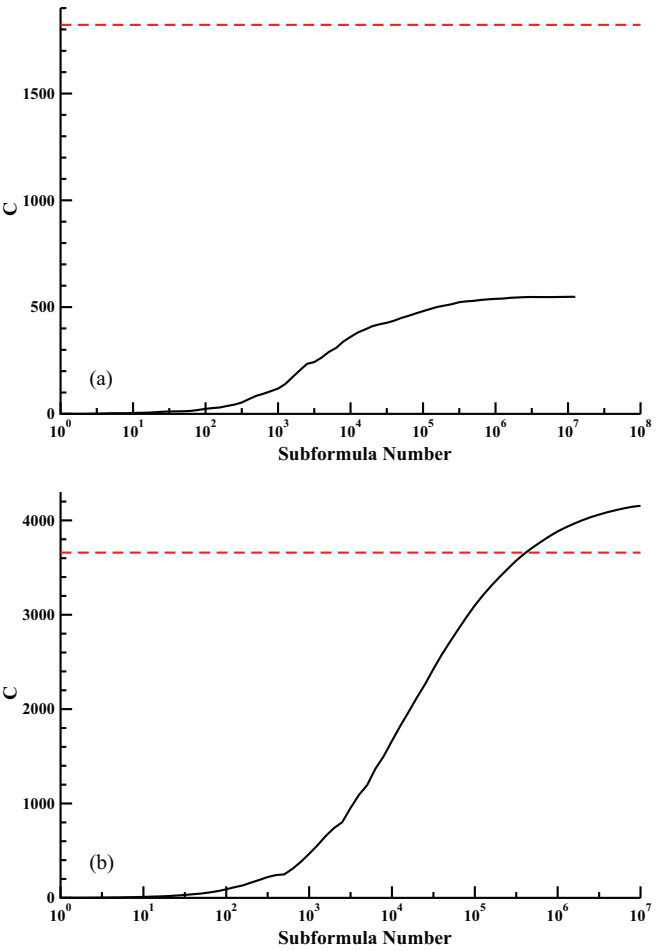

FIG. 3. (Color online) The evolution of witness value C as the number of randomly sampled subformulas t increases. The investigated random 3-SAT instance has variable number $N = 100$ and clause number $M = 10\,000$ in (A) and $M = 40\,000$ in (B). The horizontal dashed lines in (A) and (B) mark the position of $M_2^{\rm upp}$. The control parameter γ of the random sampling algorithm is set to $\gamma = 0.5$.

The above analysis suggests that for random 3-SAT instances with clause density $\alpha > N$, it is relatively easy to construct UNSAT witnesses. However, for clause density sublinear in N, it is very hard to construct UNSAT witnesses through the above random process.

The performance of this random construction process, with $\gamma = 0.5$, is demonstrated in Fig. 4 for random 3-SAT formulas with clause density $\alpha = cN$. This figure shows that for clause density scales linear with variable number N, the prefactor c needs to be greater than $c \approx 2.5$ for the random sampling algorithm to find FKO witnesses.

The random sampling algorithm is therefore very inefficient in obtaining FKO witnesses. For clause density α linear in N, other local refutation algorithms are more efficient. For example, a simple 2-SAT refutation algorithm goes as follows. First, a seed set of size s is chosen, which contains the s variables of the highest degrees. Each of the 2^s spin assignments of these s variables will induce a 2-SAT subformula, and we can check whether this 2-SAT subformula is satisfiable or not. If all these 2^s-induced 2-SAT subformulas are UNSAT, then the

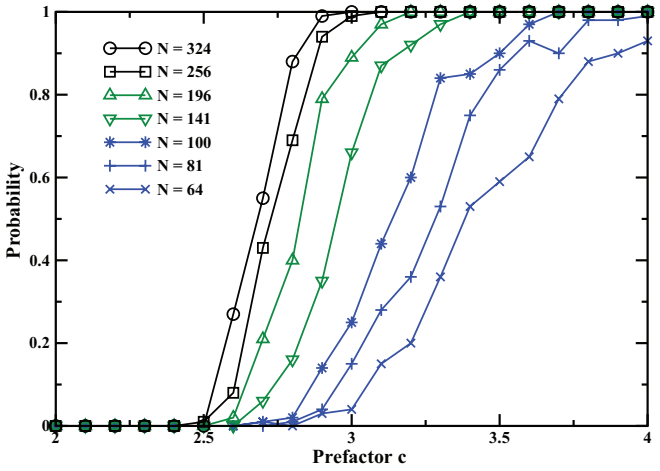

FIG. 4. (Color online) The probability of FKO witness being found in a single run of the random sampling process. Each data point was obtained by simulating ten random 3-SAT instances with N variables and $M = cN^2$ clauses. Different curves correspond to different variable numbers N.

original 3-SAT formula cannot be satisfied. The number of clauses in the induced 2-SAT subformula is larger than $\frac{3}{2}s\alpha$, and the number of variables is at most N. Since a random 2-SAT formula is very likely to be unsatisfiable if the number of clauses exceeds the number of variables, then we see that the simple 2-SAT refutation algorithm has a high probability of success if $\alpha > \frac{2}{3s}N$. The simulation results shown in Fig. 5 confirm this expectation.

C. Focused local search

The subformulas constructed by the random sampling algorithm are very sparse. Most of the loops in such a subformula are long-ranged, with lengths scaling logarithmically with the number of variables. We now consider another construction

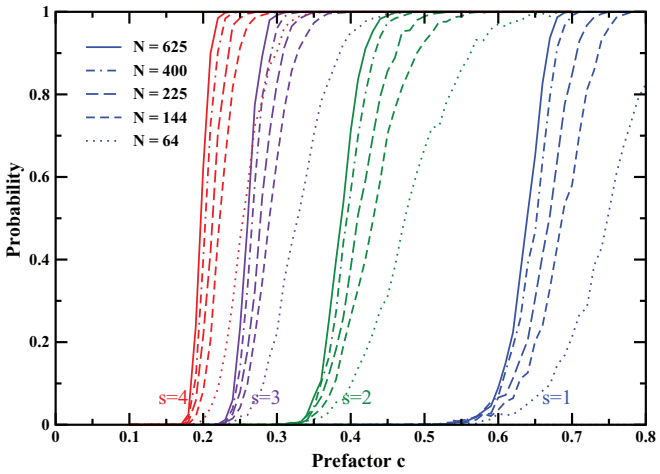

FIG. 5. (Color online) The probability of a random 3-SAT formula with N variables and cN^2 clauses (clause density $\alpha = cN$) being proven to be UNSAT by the 2-SAT refutation algorithm. The seed size s is fixed to $s = 1$, $s = 2$, $s = 3$, and $s = 4$ in the four sets of simulation curves. Each curve is the average over ten random instances.

strategy, namely, focused local search. The goal of this strategy is to construct 3-XORSAT unsatisfiable subformulas with only short loops.

The details of the focused local search algorithm are as follows:

(0) The used set U of clauses is initialized as empty.

(1) Arbitrarily choose a clause a that does not belong to the set U. This clause and all its attached three vertices form the "system" I. Any clause b that is connected to the "system" by at least one edge and is not in U belongs to the "boundary," B.

(2) In the "boundary" B some of the clauses have more connections to the "system" than the other clauses. Randomly choose a clause c in the "boundary" that has the maximal number of connections with the "system" (i.e., the number of edges to the "system" is the maximal among all the clauses in the "boundary"). Include clause c and all its attached vertices to the "system," and add clause c to the set U. The "boundary" B is then updated. Clause c is then removed from B, and all the clauses that are connected to the "system" and do not belong to set U are added to B.

(3) Check whether the "system" is 3-XORSAT satisfiable; if yes and the "boundary" B is not empty, go back to step **2**. If the "system" is 3-XORSAT unsatisfiable, then go to step **4**. If the "system" is still satisfiable but the boundary B becomes empty, then stop and output "construction failed".

(4) After an unsatisfiable 3-XORSAT subformula is obtained, the number of unsatisfied clauses in this subformula is 1. We then prune the subformula by removing unnecessary clauses so that an unsatisfiable core subformula is obtained. In the pruning process, basically we test (in a random order) whether each clause can be removed from the subformula without making it 3-XORSAT satisfiable. If a clause is removed from the subformula, it is also removed from the used clause set U.

(5) Update the subformula number t to $t + 1$. If $t \leqslant M_2^{\mathrm{upp}}$, go back to step **1**; otherwise stop and output "UNSAT witness found".

In the above-mentioned focused local search algorithm, each clause can only appear in $S = 1$ subformula. Therefore all the constructed subformulas are disjoint in the sense that they do not share any clauses. Figure 6 shows the performance of this focused local search algorithm on a set of random 3-SAT instances with $N = 1000$ variables. As the clause density α increases around a certain threshold value α_0, the probability of finding a FKO witness increases quickly from 0 to 1. The simulation data can be well fitted by a sigmoidal curve

$$P(\alpha) = \frac{1}{1 + \exp\left(-\frac{\alpha - \alpha_0}{\Delta}\right)}, \tag{24}$$

where the parameter Δ controls the slope of the sigmoidal curve. At $\alpha = \alpha_0$ the focused local search algorithm has $1/2$ probability of successfully constructing a FKO witness for a random 3-SAT instance of N variables. We therefore take α_0 as a quantitative measure of the algorithmic performance. The scaling of α_0 with variable number N is shown in Fig. 7. We find that

$$\alpha_0 \approx cN^b, \tag{25}$$

with exponent $b \approx 0.589$ and prefactor $c \approx 8.0$. The exponent b is much larger than the value of 0.4, which was predicted

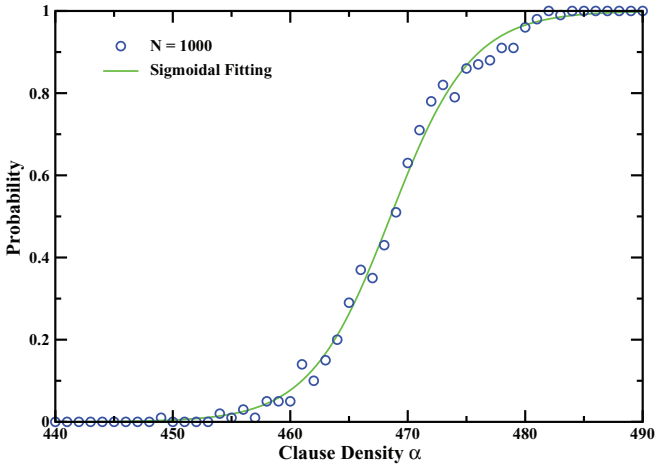

FIG. 6. (Color online) The probability of FKO witness being found in a single run of the focused local search process (control parameter $S = 1$) for random 3-SAT instances with $N = 1000$ variables and $M = \alpha N$ clauses. Each data point was obtained by simulating 100 random 3-SAT instances. The solid line is a sigmoidal fitting curve with parameters $\alpha_0 = 468.54 \pm 0.09$ and $\Delta = 3.44 \pm 0.08$.

to be achievable at least by a weak exponential-complexity algorithm [16]. It is also larger than the value of 0.5 achieved by the spectral methods [13–15], which consider both the local and the global structural properties of the random 3-SAT problem. At the moment we do not have any analytical argument with regard to the value of b of the focused local search algorithm.

We find that if we allow each clause to be present in $S \geqslant 2$ subformulas, the performance of the focused local search algorithm will be improved. The scaling behaviors of this modified algorithm with $S = 2$ and $S = 4$ are also shown in Fig. 7. The

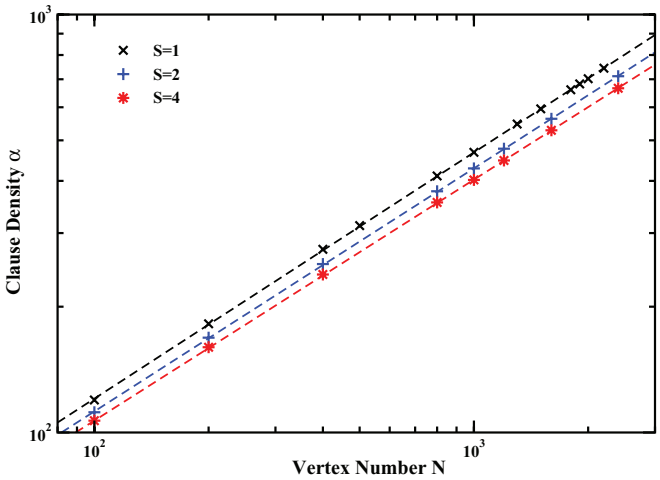

FIG. 7. (Color online) Scaling behavior between variable number N and the characteristic clause density $\alpha = \alpha_0$ of the focused local search algorithm. The control parameter of the focused local search algorithm is S. The dashed lines are fitting curves of the form $\alpha_0 = c \times N^b$. The fitting parameters are $c = 8.0 \pm 0.1$ and $b = 0.589 \pm 0.002$ (top, $S = 1$); $c = 7.7 \pm 0.1$ and $b = 0.582 \pm 0.002$ (middle, $S = 2$); and $c = 7.5 \pm 0.1$ and $b = 0.577 \pm 0.002$ (bottom, $S = 4$).

simulation data suggest that both the scaling exponent b and the prefactor c decrease slightly with S. As we have not yet performed systematic simulations for large values of S, we do not know to what extent the exponent b can be reduced.

V. CONCLUSION AND DISCUSSION

In this paper, we demonstrated through mean-field calculations that unsatisfiability of random 3-SAT by reduction to random 3-XORSAT is possible for instances with constant clause density $\alpha > 19$. On the other hand, for $\alpha < 19$ we conclude that it is *impossible* to refute a random 3-SAT formula through such an approach. The reduction and a lower bound on the 3-XORSAT ground-state energy is a witness of unsatisfiability. We investigated the empirical performance of two algorithms to find Feige-Kim-Ofek (FKO) witnesses [16]. A naive random sampling algorithm is only able to construct such witnesses for random 3-SAT instances with clause density $\alpha > cN$ (where N is the number of variables and c is a constant). The focused local search algorithm has much better performances; it works for $\alpha > cN^b$ with $b \approx 0.59$. The value of the exponent b can be further decreased by enlarging the control parameter S of the focused local search algorithm. It would be interesting to systematically investigate the relationship between b and S by computer simulations in a future work.

The essence of the FKO witness is to construct a rigorous lower bound for the ground-state energy E_0^{xor} of the 3-XORSAT formula (4). The tighter this lower bound to E_0^{xor} is, the better the refutation power of this witness approach. A very big theoretical and algorithmic challenge is to obtain a good lower bound for the ground-state energy of the 3-XORSAT problem. For the 3-SAT problem, Håstad proved in Ref. [25] that no algorithm is guaranteed to construct spin assignments that can satisfy more than $(7/8)M_{\text{opt}}$ clauses in polynomial time (M_{opt} being the maximal number clauses that can be simultaneously satisfied), unless $P = NP$. This actually gives an upper bound on the ground-state energy of the 3-SAT problem. This upper bound can be converted to an upper bound for E_0^{xor} of the 3-XORSAT problem. But we do not know any energy lower bound for the 3-XORSAT problem, whose value is *proportional to* the clause density α. If such an energy lower bound can be verified algorithmically, then the FKO witness approach could succeed for the 3-SAT problem with constant α.

The 3-XORSAT energy lower-bound C as obtained from Eq. (19) does not scale linearly with the clause density α but only sublinearly. One possible way of improving the value of C is as follows. For each constructed 3-XORSAT unsatisfiable subformula f, we assign a properly chosen real-valued weight w_f. Correspondingly, the counting number d_a of each clause a is modified as

$$d_a = \sum_{\{f|a\in f\}} w_f, \tag{26}$$

where the summation is over all the subformulas f that contain clause a. Then Eq. (19) is changed into

$$\sum_{a=1}^{C} d^{(a)} \geqslant \sum_{f} w_f. \tag{27}$$

When all the weights $w_f = 1$, then Eq. (27) reduces to Eq. (19). By optimizing the choices of the subformula weights $\{w_f\}$ we expect that a better energy lower-bound C can be obtained from Eq. (27).

The counting number d_a of each clause a can also be considered as a real-valued parameter whose value can be freely adjusted. Then the weight of each constructed subformula f is defined as $w_f = \min_{a\in f} d_a$ (i.e., the lowest value of d_a over all the clauses of f). Another better energy lower-bound C might be achievable by optimizing the choices of $\{d_a\}$.

A systematic exploration of these two reweighting schemes and other possible extensions will be carried out in a separate study.

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APPENDIX: ESTIMATING THE GLOBAL MINIMUM ENERGY DENSITY BY THE MEAN-FIELD CAVITY METHOD

To obtain the value of $M_2^{\max}$ defined by Eq. (16), we need to calculate the global minimum of the following energy function:

$$E(\underline{\sigma}) = \sum_{a=1}^{M} E_a = \sum_{a=1}^{M} \delta\left(\left|\sum_{j\in\partial a} J_a^j \sigma_j\right| - 3\right). \tag{A1}$$

This energy $E(\underline{\sigma})$ is contributed by M clauses. The energy E_a of clause a is unity if $\sum_{j\in\partial a} J_a^j \sigma_j = 3$ or $= -3$; otherwise this energy is zero. The global minimum of (A1) can be estimated through the mean-field first-step replica-symmetry-breaking (1RSB) spin glass theory [19]. Here we give a brief description of the technical details. For readers unfamiliar with the mean-field spin glass theory, all the equations mentioned below can also be derived from the mathematical framework of partition function expansion [26,27].

Consider all the configurations that are local or global minima of the energy function (A1). It is assumed that these configurations can be grouped into many well-separated clusters, with each cluster $\mathcal{C}$ containing a set of minimum-energy configurations that have the same energy $E_{\mathcal{C}}$ and are similar to each other. A grand partition function at the level of minimum-energy configuration clusters is defined as $\Xi \equiv \sum_{\mathcal{C}} e^{-yE_{\mathcal{C}}}$, where y is a reweighting parameter. The grand free energy is then $G \equiv -\frac{1}{y}\ln\Xi$, and it is calculated through

$$G = \sum_{i=1}^{N} g_{i+\partial i} - \sum_{a=1}^{M} (|\partial a| - 1) g_a + \Delta G, \tag{A2}$$

where $g_{i+\partial i}$ is the contribution from vertex i and all its connected clauses ($a \in \partial i$), g_a is the contribution from a single clause a (the value of $|\partial a|$ is equal to 3 in our case), and ΔG is the total loop correction contributions. Because of the absence of short loops in a random factor graph, the correction contribution ΔG can be safely neglected in the thermodynamic limit of $N \to \infty$ [26,27].

To calculate g_a, let us remove clause a from the energy function (A1) to get a cavity system. For each minimal-energy configuration cluster of this cavity system, a coarse-grained frozen state $f_{i\to a}$ for a vertex $i \in \partial a$ is defined as follows: If the spin σ_i of vertex i is always $+1$ in all the configurations of this cluster, its frozen state is $f_{i\to a} = +1$; if $\sigma \equiv -1$ in all the configurations of this cluster, its frozen state is $f_{i\to a} = -1$; otherwise its frozen state is $f_{i\to a} = 0$ (unfrozen). Denote by $p_{i\to a}(f_{i\to a})$ the probability distribution of $f_{i\to a}$ over all the configuration clusters of the cavity system. After clause a is added to the cavity system to form the complete system, the change g_a in the grand free energy is expressed as

$$g_a = -\frac{1}{y}\ln\left[\prod_{i\in\partial a}\sum_{f_{i\to a}\in\{-1,0,+1\}} p_{i\to a}(f_{i\to a}) \times \exp\left[-y\delta\left(\left|\sum_{i\in\partial a} J_a^i f_{i\to a}\right| - 3\right)\right]\right] \tag{A3}$$

$$= -\frac{1}{y}\ln\left[1 - (1-e^{-y})\left[\prod_{i\in\partial a} p_{i\to a}\left(J_a^i\right) + \prod_{i\in\partial a} p_{i\to a}\left(-J_a^i\right)\right]\right]. \tag{A4}$$

In Eq. (A3), $\delta(|\sum_{i\in\partial a} J_a^i f_{i\to a}| - 3)$ is the increase to the minimal energy of a configuration cluster caused by the addition of clause a.

We can also remove vertex i and all the clauses $a \in \partial i$ from the energy function (A1) to get another cavity system. The change in the grand free energy caused by adding these removed vertex and clauses back to the system is

$$g_{i+\partial i} = -\frac{1}{y}\ln\left[\prod_{a\in\partial i}\prod_{j\in\partial a\setminus i}\sum_{f_{j\to a}\in\{-1,0,+1\}} p_{j\to a}(f_{j\to a}) \times \exp\left[-y\min\left(\sum_{a\in\partial i}\delta(u_{a\to i} - 1), \sum_{a\in\partial i}\delta(u_{a\to i} + 1)\right)\right]\right], \tag{A5}$$

where $u_{a\to i}$ is a warning message from clause a to vertex i with the expression

$$w_{a\to i}=\begin{cases}-J_a^i, & \text{for } \sum_{j\in\partial a\setminus i} J_a^j f_{j\to a}=2,\\ J_a^i, & \text{for } \sum_{j\in\partial a\setminus i} J_a^j f_{j\to a}=-2,\\ 0, & \text{for } \left|\sum_{j\in\partial a\setminus i} J_a^j f_{j\to a}\right|\leqslant 1.\end{cases} \tag{A6}$$

The integer number $\min[\sum_{a\in\partial i}\delta(u_{a\to i}-1),\sum_{a\in\partial i}\delta(u_{a\to i}+1)]$ is the increase to the minimal energy of a configuration cluster caused by the addition of vertex i and the set of clauses ∂i.

The grand free energy G should be stationary with respect to the set of probability functions $\{p_{i\to a}(f_{i\to a})\}$. The requirement that $\frac{\delta G}{\delta p_{i\to a}}=0$ leads to the following self-consistent equation:

$$p_{i\to a}(f_{i\to a})=\frac{\prod_{b\in\partial i\setminus a}\prod_{j\in\partial b\setminus i}\sum_{f_{j\to b}\in\{-1,0,+1\}} p_{j\to b}(f_{j\to b})\delta\left[f_{i\to a}-\mathrm{sgn}(w^+_{i\to a}-w^-_{i\to a})\right]e^{-y\min(w^+_{i\to a},w^-_{i\to a})}}{\prod_{b\in\partial i\setminus a}\prod_{j\in\partial b\setminus i}\sum_{f_{j\to b}\in\{-1,0,+1\}} p_{j\to b}(f_{j\to b})e^{-y\min(w^+_{i\to a},w^-_{i\to a})}}, \tag{A7}$$

where $w^+_{i\to a}\equiv\sum_{b\in\partial i\setminus a}\delta(u_{b\to i}-1)$, $w^-_{i\to a}\equiv\sum_{b\in\partial i\setminus a}\delta(u_{b\to i}+1)$, and the function $\mathrm{sgn}(x)$ is defined as $\mathrm{sgn}(x)=1$ if $x>0$, $\mathrm{sgn}(x)=-1$ if $x<0$, and $\mathrm{sgn}(x)=0$ if $x=0$.

At a given value of reweighting parameter y, we can iterate the set of message-passing equations (A7) to reach a fixed point. Then the free energy can be computed through Eq. (A2) with ΔG being set to zero. The mean minimal energy is then computed through $\langle E_{\mathcal{C}}\rangle\equiv\frac{\partial(yG)}{\partial y}$, and the entropy density Σ of configuration clusters contributing to this minimal energy density can also be computed through $\Sigma=y\frac{\langle E_{\mathcal{C}}\rangle-G}{N}$. As the reweighting parameter y increases, the mean minimal energy density value decreases. At a critical value $y=y^*$ the complexity Σ changes from positive to negative. The mean minimal energy density obtained at $y=y^*$ is then regarded as the energy density of the global energy minimum.

The above mean-field theory is applicable to a given random factor graph. If we are interested in the ensemble-averaged property, the calculation will be simpler. We just need to update a large population of probability profiles $\{p_{i\to a}(f_{i\to a})\}$ using Eq. (A7). During the updating process the average value of $g_{i+\partial i}$ over all the different vertices i and the average value of g_a over all the different clauses a can be obtained simultaneously.

The mean-field equations for the 3-XORSAT problem (4) can be written down in a similar way (see also [19]).

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