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Exhaustive enumeration unveils clustering and freezing in the random 3-satisfiability problem

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We study geometrical properties of the complete set of solutions of the random 3-satisfiability problem. We show that even for moderate system sizes the number of clusters corresponds surprisingly well with the theoretic asymptotic prediction. We locate the freezing transition in the space of solutions, which has been conjectured to be relevant in explaining the onset of computational hardness in random constraint satisfaction problems.

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Satisfiability (SAT) is one of the most important problems in theoretical computer science. It was the first problem shown to be NP-complete [1,2], and it is of central relevance in various practical applications, including artificial intelligence, planning, hardware and electronic design, automation, verification, and more. It can thus be pictorially thought of as the Ising model of computer science. Ensembles of randomly generated SAT instances emerged in computer science as a way of evaluating algorithmic performance and addressing questions regarding the average case complexity.

An instance of a random K-SAT problem consists of N Boolean variables and M clauses. Each clause contains a subset of K distinct variables chosen uniformly at random, and each clause forbids one random assignment of the K variables out of 2^K possible ones. The problem is *satisfiable* if there exists an assignment of variables that simultaneously satisfies all clauses, and we call such an assignment a *solution* to the problem. When the density of constraints, $\alpha = M/N$, is increased, the formulas become less likely to be satisfiable. In the thermodynamical limit there is a sharp transition from a phase in which the formulas are almost surely satisfiable to a phase where they are almost surely unsatisfiable. The existence of this transition is partly established rigorously [3]. It is also a well-known empirical result that the hardest instances are found near to this threshold [4–6].

Random K-SAT has attracted the interest of statistical physicists because of its equivalence to mean-field spin glasses [7]. Indeed, the problem can be rephrased as minimizing a spin-glass-like energy function which counts the number of violated clauses. The results and insights coming from this equivalence are remarkable. The satisfiability threshold and other phase transitions in the structure of solutions are described in [8–10]. In particular, it was shown that for $K \geqslant 3$ the space of solutions for highly constrained but still satisfiable instances splits into exponentially many clusters and in some cases this clustering has been rigorously confirmed [11,12]. The so-called freezing of variables in clusters is another rich concept studied recently [13–15]. However, a detailed understanding of how the clustering or freezing of solutions affects the average computational hardness is still one of the most interesting open problems in the field.

Since the exact statistical physics solution of the random satisfiability problem appeared [9,16], dozens of directly related articles followed. Mathematicians and computer scientists nowadays regard these analytical works as a rich source of results which are mostly inaccessible to current probabilistic methods. Yet none of these works tried to compare the analytical asymptotic predictions to numerical simulations on a quantitative level and numerical investigations mostly concentrated on performance analysis of satisfiability solvers. Therefore the relevance of the asymptotic predictions for systems of practical sizes, which in computer science are not at the scale of the Avogadro number, remained almost untouched. Our Rapid Communication aims at filling this gap and to encouraging further investigation in this direction. We use conceptually relatively simple numerical techniques and yet obtain nontrivial results. We present two of our most interesting findings. The first is a quantitative comparison between the number of clusters of solutions (glassy states) and its analytical prediction [9,16–18]. The second is the location of the freezing transition, which was recently suggested to be responsible for the computational hardness of the random satisfiability problem [14,19,20], but not yet computed in the 3-SAT problem.

In the physics of glassy systems, clusters correspond to pure thermodynamical states and have been described in the literature about glasses and spin glasses for more than one-quarter of a century [7]. A formal definition of clusters in K-SAT as extremal Gibbs measures was given recently in [10]. We will refer to these as the *cavity clusters*. It is not known, however, how to adapt this definition to instances of finite size. In this work, we adopt a definition of clusters as connected components in a graph where each solution is a vertex and where edges connect solutions that differ in only one variable.[1] This definition is applicable to any finite instance of the K-SAT problem. It is, however, unable to describe purely entropic barriers, and it is thus most likely not

[1]This distance-1-separated clusters are in K-SAT asymptotically equivalent to any finite-distance-separated clusters. It is, however, not known if they are equivalent also to "any subextensive-distance"-separated clusters.

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asymptotically equivalent to the definition of the cavity clusters, yet it reproduces many of their properties.

In order to shed light on the relation between cavity clusters and connected-component clusters we now introduce the procedure called *whitening* and the concept of frozen variables. *Whitening of a solution* in K-SAT is defined in the following way [21]: start with the solution, assign iteratively a "$*$" (joker) to variables which belong only to clauses which are already satisfied by another variable or already contain a $*$ variable.[2] The fixed point of this procedure is called a *whitening core*.[3] A variable is said to be *frozen* in a set of solutions if it takes only one value (either 0 or 1) in all the solutions in the set. Note that if the satisfiability threshold is sharp, there cannot be a finite fraction of variables frozen in all the solutions in the satisfiable region [22]. On the other hand, variables might be frozen in the individual clusters. According to the cavity method [23,24] this is indeed the case and freezing of clusters has been studied in [13–15].

According to the cavity method [23,24] there is a deep connection between frozen variables and the whitening core: if the one-step replica-symmetric solution is correct, then on large typical instances the set of frozen variables in the cavity cluster and the non-$*$ part of the whitening core are identical [9]. Thus the whitening cores of all solutions belonging to one cavity cluster are identical. This also holds for the connected-component clusters: Indeed, two solutions that differ in a single variable have the same whitening core since the whitening can be started from that specific variable. Further, variables belonging to the whitening core must be frozen in the connected-component cluster; the opposite implication is in general not true.

Two additional remarks about clusters are important. First, whitening cores are sometimes wrongly identified with clusters. Note that solutions having the all-$*$ whitening core typically do not belong to the same cluster. We have not found any general argument why two different connected-component clusters could not have the same non-all-$*$ whitening core, but we have not observed any such case in our data. Second, it seems that all known heuristic algorithms need an exponential time to find solutions with a nontrivial (not all-$*$) whitening core; see, e.g., [14,25,26]. This motivates our study of the *freezing transition* α_f. It is defined as the smallest density of constraints α such that all solutions belong to frozen clusters; i.e., their whitening core is not made from all-$*$. We use the whitening core instead of the real set of frozen variables, because in small instances there are almost always at least a few frozen variables. The existence of the frozen phase was proven in the thermodynamical limit for $K \geqslant 9$ near to the satisfiability threshold in [12]. Several theoretical investigations of a related rigidity transition, where clusters which contain almost all the solution become frozen, can be found in [13–15]. But as long as soft clusters exist, some algorithms may be able to find them, as

[2]In a general constraint satisfaction problem the whitening must be defined via the warning propagation. Whitening is in the literature referred also as peeling [25] or coarsening [12].

[3]A whitening core is also referred to as a core [12,25], or a true cover [27].

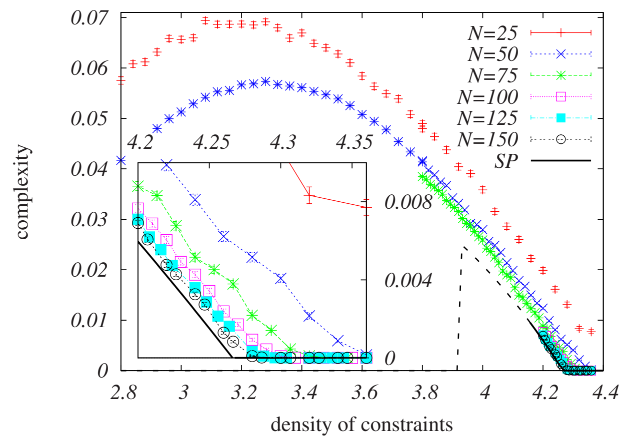

FIG. 1. (Color online) The average complexity function, logarithm of the number of connected-component clusters divided by N, for different system sizes compared to the asymptotic prediction [16,18], which is reliable (stable) only for $\alpha > 4.15$ [17]. Note that all the numerical curves continue to lower values of α than plotted and asymptotically will not stop at $\alpha = 3.92$ or at $\alpha = 3.86$.

shown in [20]. A related numerical study [27] investigates the size dependence of the fraction of frozen solutions at $\alpha = 4.20 < \alpha_f$.

We generate instances of the random 3-SAT problem with N variables and M clauses using the MAKEWFF program [28]. The number of solutions is then calculated using the exhaustive search method RELSAT [29]. The complete set of solutions is clustered through *breath first search*: We order the $\mathcal{N}$ solutions in binary lexical order. Further, for all the solutions we generate all the N neighboring configurations, search them in the list, and if found, concatenate the two in the same cluster, resulting in an algorithmic complexity of $O(\mathcal{N} \ln^2 \mathcal{N})$, considering that $\ln \mathcal{N} \approx N$.

In order to obtain information about clusters in a typical formula with N variables and M clauses, we count the number of solutions in $A = 999$ such random formulas and select the median instance in terms of the number of solutions on which we then count the number of clusters, $\mathcal{S}$. This is repeated $B = 1000$ times. The complexity function $\Sigma(N) = \langle \ln \mathcal{S} \rangle / N$ is then computed as the average of the logarithm of the number of clusters divided by the system size N. If the median instance is unsatisfiable, it contributes a zero value to the average; this does not have an influence on the asymptotic value. Taking the median has two important advantages: first, we avoid rare formulas with very many solutions which are numerically intractable; second, the complexity converges very fast to zero in the unsatisfiable region.

The result is plotted in Fig. 1 and compared with the asymptotic complexity function computed from the survey propagation equations, which in 3-SAT gives a nonzero result for $\alpha > 3.92$ [16,18], but is reliable only for $\alpha > 4.15$ [17]. The agreement is remarkably good, in particular around the satisfiability threshold $\alpha_s = 4.267$ [9,18]. It was discussed in [10], and shown numerically also in [27], that clusters exist even for $\alpha < 3.92$. We indeed do not see anything in particular happening at $\alpha = 3.92$. Below the clustering transition, $\alpha < 3.86$, however, the largest cavity cluster should contain almost all the solutions [10]. We see a corresponding

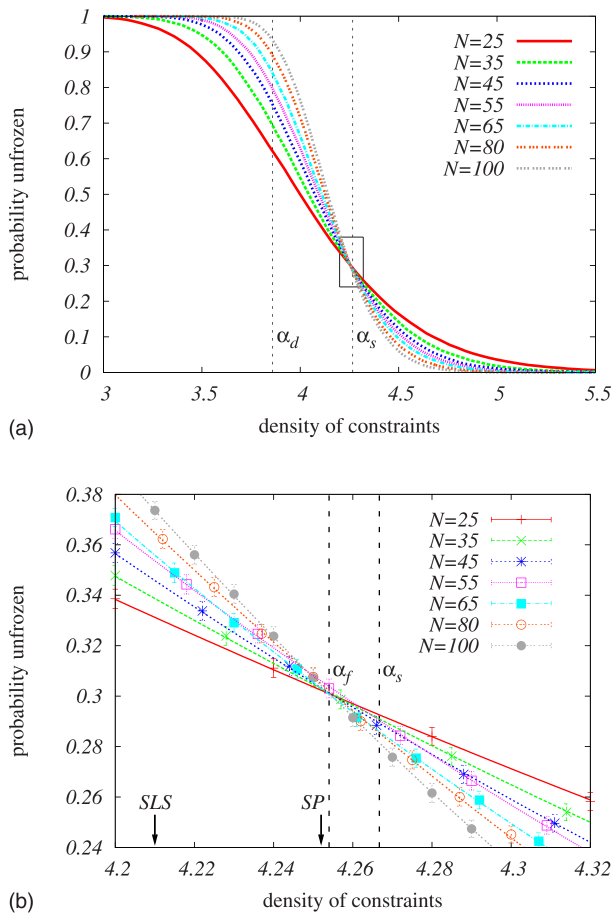

FIG. 2. (Color online) (a) probability that there exists an unfrozen solution as a function of the constraint density α for different system sizes. The clustering [10] and satisfiability [9] transitions are marked for comparison. (a) A 1:20 zoom-in on the critical (crossing) point. Our estimate for the freezing transition is $\alpha_f = 4.254 \pm 0.009$. The curves are cubic fits in the interval (4,4.4). The arrows represent estimates of the limits of performance of the best known stochastic local search [26,33] and survey propagation [34,35] algorithms.

trend in the average fraction of solutions covered by the largest cluster in our data. The result of Fig. 1 can also be seen as a confirmation of the close relation between the connected-component and cavity clusters.

In order to determine the freezing transition we start with a formula of N variables and all possible clauses, and remove the clauses one by one independently at random. We mark the number of clauses M_s where the formula becomes satisfiable as well as the number of clauses $M_f \leqslant M_s$ where at least one solution starts to have an all-$*$ whitening core. We repeat B times ($B=2\times 10^4$ in Fig. 2) and compute the probabilities that a formula of M clauses is satisfiable $P_s(\alpha,N)$ and unfrozen $P_f(\alpha,N)$, respectively. Due to memory limitation, we can treat only instances which have less than 5×10^7 solutions, which limits us to system sizes $N \leqslant 100$. Our results for the satisfiability threshold are consistent with previous studies in [6,22,30]. The probability of being unfrozen, $P_f(\alpha,N)$, is shown in Fig. 2.

It is tempting to perform a scaling analysis as has been done in [6,22,30] for the satisfiability threshold. The critical exponent related to the width of the scaling window was defined via rescaling of variable α as $N^{1/\nu_s}[1-\alpha/\alpha_s(K,N)]$. Note, however, that the estimate $\nu_s = 1.5 \pm 0.1$ for 3-SAT provided in [30] is not the correct asymptotic value. It was proven in [31] that $\nu_s \geqslant 2$. Indeed, it was shown numerically in [32] that a crossover exists at sizes of order $N \approx 10^4$ in the related XOR-SAT problem. A similar situation happens for the scaling of the freezing transition, $P_f(\alpha,N)$, as the proof of [31] applies also here.[4] It would be interesting to investigate the scaling behavior on an ensemble of instances where results of [31] do not apply. Here we concentrate instead on the estimation of the critical point, which we presume not to be influenced by the crossover in the scaling. We are in a much more convenient situation than for the satisfiability transition. The crossing point for the functions $P_f(\alpha,N)$ of different system sizes seems not to depend on N, while for the satisfiability transition its size dependence is very strong [30].

We determine the value of the freezing transition as $\alpha_f = 4.254 \pm 0.009$, which is extremely close to the satisfiability threshold $\alpha_s = 4.267$ [16]. Analytical study suggests $\alpha_f > 4.25$ [36]. We expect the two transitions to be separated, $\alpha_f < \alpha_s$ [12,14,15], and Fig. 2 suggests so, but it is on the border of statistical significance. However, the main motivation to study the freezing transition is its potential connection to the onset of algorithmical hardness [14,19,20]. We thus compare its value with the estimates of performance of the best algorithms known for random 3-SAT. The leading stochastic local search algorithms work in linear time up to $\alpha = 4.21$ [26,33]. The survey propagation (SP) decimation was estimated to work up to $\alpha = 4.252$ [34]; the same point was determined as the limit of the SP reinforcement [35]. The agreement between our location of the freezing transition and the performance of SP supports strongly the conjecture that the frozen phase is hard for any known algorithm. In random 3-SAT this region is very narrow, in contrast to the situation in $K \geqslant 9$ SAT [12].

The main contribution of this work is the demonstration that the asymptotic predictions coming from the statistical physics analysis are relevant even for instances of very moderate size. In particular, we presented a numerical comparison between the number of connected-component clusters and the asymptotic prediction for the complexity function in random 3-SAT and obtain a remarkably good agreement. Furthermore, we estimate the location of the freezing transition at $\alpha_f = 4.254$, which is consistent with the performance threshold of the best known algorithms. We also show that exhaustive enumeration, despite its current size limitations, is a powerful tool to study random optimization problems: indeed the knowledge of the complete set of solutions allows us to tackle questions that are complementary to those answered by classical Monte Carlo methods.

The definitions of clusters and the whitening core that we adopted are applicable to any instance of the satisfiability problem. As such, they offer an interesting direction for fu-

[4]Theorem 1 of [31] applies to the freezing property where the bystander are clauses containing two leaves.

ture research of real-world K-SAT instances. However, the relation and eventual equivalence between the cavity and connected-component clusters are still to be substantiated. In addition, we observe that the properties related to clustering are less sensitive to finite-size effects than the ones related to the solutions themselves. This is interesting and certainly worth further investigations. Future work could also cover 2-SAT, where the solutions are much more numerous even for very small system sizes, or K-SAT with $K>3$, where larger formulas will be needed to investigate the relevant regions; however, the freezing transition is more separated from the satisfiability when K grows. The numerical location of the clustering and condensation transitions [10] is also of interest.

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