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Phase coexistence and finite-size scaling in random combinatorial problems

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Abstract

We study an exactly solvable version of the well known random Boolean satisfiability (SAT) problem, the so-called random XOR–SAT problem. Rare events are shown to affect the combinatorial 'phase diagram' leading to a coexistence of solvable and unsolvable instances of the combinatorial problem in a certain region of the parameters characterizing the model. Such instances differ by a non-extensive quantity in the ground state energy of the associated diluted spin glass model. We also show that the critical exponent ν, controlling the size of the critical window where the probability of having solutions vanishes, depends on the model parameters, shedding light on the link between random hyper-graph topology and universality classes. In the case of random SAT, a similar behaviour was conjectured to be connected to the onset of computational intractability.

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1. Introduction

The satisfaction of constrained Boolean formulae, the so-called satisfiability (SAT) problem, is a key problem of complexity theory in computer science that can be recast as an energy minimization problem (ground state search) in diluted spin glass models. Many hard computational problems have been shown to be NP-complete [1] through a polynomial mapping onto the SAT problem, which in turn was the first problem identified as NP-complete by Cook in 1971 [2].

Recently [3], the research activity has become more and more focused on the study of the random version of the SAT problem defined as follows. Consider N Boolean variables x_i, $i = 1, \ldots, N$. Call clause C the logical OR of K randomly chosen variables, each of them being negated or left unchanged with equal probabilities. Then repeat this process by drawing independently M random clauses C_σ, $\sigma = 1, \ldots, M$. The logical AND of all clauses

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$\mathcal{F}$ is said to be satisfiable if there exists a logical assignment of the $\{x_i\}$ evaluating $\mathcal{F}$ to true, unsatisfiable otherwise.

Numerical experiments have concentrated upon the study of the probability $P_N(\gamma, K)$ that a given $\mathcal{F}$ including $M = \gamma N$ clauses be satisfiable. For large sizes, there appears a remarkable behaviour: $P_\infty(\gamma, K)$ seems to be unity for $\gamma < \gamma_c(K)$ and vanishes for $\gamma > \gamma_c(K)$ [4, 5]. Such an abrupt threshold behaviour, separating a so-called SAT phase from an UNSAT one, has indeed been rigorously confirmed for 2-SAT, which is in P, with $\gamma_c(2) = 1$ [6]. For $K \geqslant 3$, K-SAT is NP-complete and much less is known. The existence of a sharp transition has not been rigorously proven yet but relatively good estimates of the thresholds have been found: $\gamma_c(3) \simeq 4.2$–4.3 [7]. Moreover, some rigorous lower and upper bounds to $\gamma_c(3)$ have been established [7].

The interest in random K-SAT arises from the fact that it has been observed numerically that hard random instances are created when the problems are critically constrained, i.e. close to the SAT/UNSAT phase boundary [3, 4]. The study of such hard instances represents a theoretical challenge towards a concrete understanding of complexity and the analysis of algorithms. Moreover, hard random instances are also a testbed for the optimization of heuristic (incomplete) search procedures which are widely used in practice.

The statistical mechanics study of random K-SAT has provided some geometrical understanding of the onset of complexity at the phase transition through the introduction of a functional order parameter which describes the geometrical structure of the space of solutions. The nature of the SAT/UNSAT transition for the different values of K appears to be a particularly relevant prediction [8]. The SAT/UNSAT transition is accompanied by a smooth (respectively abrupt) change in the structure of the solutions of the 2-SAT (resp. 3-SAT) problem. More specifically, at the phase boundary a finite fraction of the variables become fully constrained while the entropy density remains finite. Such a fraction of frozen variables (i.e. those variables which take the same value in all solutions) may undergo a continuous (2-SAT) or discontinuous (3-SAT) growth at the critical point. This discrepancy is responsible for the difference of typical complexities of both models recently observed in numerical studies. The typical solving time of search algorithms displays an easy–hard pattern as a function of γ with a peak of complexity close to the threshold. The peak in search cost seems to scale polynomially with N for the 2-SAT problem and exponentially with N in the 3-SAT case. From an intuitive point of view, the search for solutions ought to be more time-consuming in the presence of a finite fraction of fully quenched variables since the exact determination of the latter requires an almost exhaustive enumeration of their configurations.

To test this conjecture, a mixed $2+p$ model has been proposed, including a fraction p (resp. $1-p$) of clauses of length two (resp. three) and thus interpolating between the 2-SAT ($p = 0$) and 3-SAT ($p = 1$) problems. The statistical mechanics analysis predicts that the SAT/UNSAT transition becomes abrupt when $p > p_0 \simeq 0.4$ [8–11]. Precise numerical simulations support the conjecture that the polynomial/exponential crossover occurs at the same critical p_0. Though the problem is both critical ($\gamma_c = 1/(1-p)$ for $p < p_0$) and NP-complete for any $p > 0$, it is only when the phase transition becomes of the same type as of the 3-SAT case that hardness shows up. An additional argument in favour of this conclusion is given by the analysis of the finite-size effects on $P_N(\gamma, K)$ and the emergence of some universality for $p < p_0$. A detailed account of these findings may be found in [8–12]. For $p < p_0$ the exponent ν, which describes the shrinking of the critical window where the transition takes place, is observed to remain constant and close to the value expected for 2-SAT. The critical behaviour is the same for the percolation transition in random graphs (see also [13]). For $p > p_0$ the size of the window shrinks following some p-dependent exponents toward its statistical lower bound [14] but numerical data did not allow any precise estimate.

In this paper, we study an exactly solvable version of the random $2+p$ SAT model which displays new features and allows us to settle the issue of universality of the critical exponents. The threshold of the model can be computed exactly as a function of the mixing parameter p in the whole range $p \in [0, 1]$. Rare events are found to be dominant also in the low-γ phase, where a coexistence of satisfiable and unsatisfiable instances is found. A detailed analysis for the $p = 1$ case can be found in [15].

The existence of a global—polynomial time—algorithm for determining SAT allows us to perform a finite-size scaling analysis around the exactly known critical points over huge samples and to show that indeed the exponent controlling the size of the critical window ceases to maintain its constant value $\nu = 3$ and becomes dependent on p as soon as the phase transition becomes discontinuous, i.e. for $p > p_0 = 0.25$. Above p_0 and below $p_1 \sim 0.5$, the exponent ν takes intermediate values between 3 and 2. Finally, above p_1 the critical window is determined by the statistical fluctuations of the quenched disorder [14] and so $\nu = 2$.

2. Model definition and outline of some results

The model we study can be viewed as the mixed $2+p$ extension of the 3-*hyper-SAT* (hSAT) model discussed in [15], as much as the $2+p$ SAT [8] is an extension of the usual K-SAT model. In computer science literature the hSAT model is also named XOR–SAT and its critical behaviour is considered an open issue [16]. Given a set of N Boolean variables $\{x_i = 0, 1\}_{i=1,\dots,N}$ we can write an instance of our model as follows. Firstly, we define the elementary constraints (a mixture of 4- and 2-clauses sets with 50% satisfying assignments):

$$\begin{aligned} C(ijk|+1) &= (x_i \vee x_j \vee x_k) \wedge (x_i \vee \bar{x}_j \vee \bar{x}_k) \wedge (\bar{x}_i \vee x_j \vee \bar{x}_k) \wedge (\bar{x}_i \vee \bar{x}_j \vee x_k) \\ C(ijk|-1) &= (\bar{x}_i \vee \bar{x}_j \vee \bar{x}_k) \wedge (\bar{x}_i \vee x_j \vee x_k) \wedge (x_i \vee \bar{x}_j \vee x_k) \wedge (x_i \vee x_j \vee \bar{x}_k) \end{aligned} \tag{1}$$

for the 3-hSAT part, and

$$\begin{aligned} C(ij|+1) &= (x_i \vee \bar{x}_j) \wedge (\bar{x}_i \vee x_j) \\ C(ij|-1) &= (x_i \vee x_j) \wedge (\bar{x}_i \vee \bar{x}_j) \end{aligned} \tag{2}$$

for the 2-hSAT part. $\wedge$ and $\vee$ are the logical AND and OR operations respectively and the overbar is the logical negation. A more compact definition can be achieved by the use of the exclusive OR operator $\oplus$: e.g. $C(ijk|+1) = x_i \oplus x_j \oplus x_k$. Then, we randomly choose two independent sets E_3 and E_2 of pM triples $\{i, j, k\}$ and $(1-p)M$ couples $\{i, j\}$ among the N possible indices and respectively pM and $(1-p)M$ associated unbiased and independent random variables $T_{ijk} = \pm 1$ and $J_{ij} = \pm 1$, and we construct a Boolean expression in conjunctive normal form (CNF) as

$$F = \bigwedge_{\{i,j,k\} \in E_3} C(ijk|T_{ijk}) \bigwedge_{\{i,j\} \in E_2} C(ij|J_{ij}). \tag{3}$$

As in [15], we can build a *satisfiable* version of the model choosing clauses only of the $C(ij|+1)$ and $C(ijk|+1)$ type. For $p < p_0$ the problem is easily solved by local and global algorithms, whereas interesting behaviours are found for $p > p_0$, where the local algorithms fail.

The above combinatorial definition can be recast in a simpler form as a minimization problem of a cost–energy function on a topological structure which is a mixture of a random graph (2-spin links) and hyper-graph (3-spin hyper-links). We end up with a diluted spin model where the Hamiltonian reads

$$H_J[\boldsymbol{S}] = M - \sum_{\{i,j,k\} \in E_3} T_{ijk}\, S_i S_j S_k - \sum_{\{i,j\} \in E_2} J_{ij}\, S_i S_j \tag{4}$$

where the S_i are binary spin variables and the the random couplings can be either ± 1 at random. The satisfiable version is nothing but the ferromagnetic model: $T_{ijk} = 1$ and $J_{ij} = 1$ for any link.

As the average connectivity γ of the underlying mixed graph grows beyond a critical value $\gamma_c(p)$, the *frustrated* model undergoes a phase transition from a mixed phase in which satisfiable instances and unsatisfiable ones coexist to a phase in which all instances are unsatisfiable. At the same $\gamma_c(p)$ the associated spin glass system undergoes a zero-temperature glass transition where frustration becomes effective and the ground state energy is no longer the lowest one (i.e. that with all the interactions satisfied). At the same critical point the *unfrustrated*, i.e. ferromagnetic, version undergoes a para–ferro transition, because the same topological constraints that drive the glass (mixed SAT/UNSAT to UNSAT) transition in the frustrated model are shown to be the ones responsible for the appearance of a nonzero value of the magnetization in the unfrustrated one [15]. We shall take advantage of such coincidence of critical lines by making the analytical calculation for the simpler ferromagnetic model.

Moreover, the nature of the phase transition changes from second to random first order, when p crosses the critical value $p_0 = 1/4$. For $p > p_0$ the critical point $\gamma_c(p)$ is preceded by a dynamical glass transition at $\gamma_d(p)$ where ergodicity breaks down and local algorithms get stuck (local algorithms are procedures which update the system configuration only by changing a finite number of variables at the same time, e.g. all single or multi spin flip dynamics, together with the usual computer science heuristic algorithms). The dynamical glass transition exists for both versions of the model [17] and corresponds to the formation of a locally stable ferromagnetic solution in the unfrustrated model [18] (the local stability is intimately related to the ergodicity breaking).

3. Statistical mechanics analysis

Following the approach of [15], we compute the free energy of the model with the replica method, exploiting the identity $\log\langle\langle Z^n\rangle\rangle = 1 + n\langle\langle \log Z\rangle\rangle + \mathrm{O}(n^2)$. The nth moment of the partition function is obtained by replicating n times the sum over the spin configurations and then averaging over the quenched disorder:

$$\langle\langle Z^n\rangle\rangle = \sum_{\boldsymbol{S}^1,\boldsymbol{S}^2,\ldots,\boldsymbol{S}^n} \left\langle\!\!\left\langle \exp\left(-\beta \sum_{a=1}^{n} H_J[\boldsymbol{S}^a]\right)\right\rangle\!\!\right\rangle. \tag{5}$$

Since each of the M clauses is independent, the probability distributions of the ferromagnetic couplings can be written as

$$\begin{aligned} P(\{T_{ijk}\}) &= \prod_{i<j<k}\left[\left(1-\frac{6\gamma p}{N^2}\right)\delta(T_{ijk}) + \frac{6\gamma p}{N^2}\delta(T_{ijk}-1)\right] \\ P(\{J_{ij}\}) &= \prod_{i<j}\left[\left(1-\frac{2\gamma(1-p)}{N}\right)\delta(J_{ij}) + \frac{2\gamma(1-p)}{N}\delta(J_{ij}-1)\right] \end{aligned} \tag{6}$$

giving the following expression for the $\langle\langle Z^n\rangle\rangle$:

$$\begin{aligned} \langle\langle Z^n\rangle\rangle = \sum_{S_i^1,S_i^2,\ldots,S_i^n} \exp\Bigg\{ &-\beta\gamma N n - \gamma N \\ &+\frac{p\gamma}{N^2}\sum_{ijk} \mathrm{e}^{\beta\sum_a S_i^a S_j^a S_k^a} + \frac{(1-p)\gamma}{N}\sum_{ij}\mathrm{e}^{\beta\sum_a S_i^a S_j^a} + \mathrm{O}(1)\Bigg\}. \end{aligned} \tag{7}$$

Introducing the occupation fractions $c(\vec{\sigma})$ (fraction of sites with replica vector $\vec{\sigma}$), one gets

$$-\beta F[c] = -\gamma(1+\beta n) - \sum_{\vec{\sigma}} c(\vec{\sigma}) \log c(\vec{\sigma}) + (1-p)\gamma \sum_{\vec{\sigma},\vec{\rho}} c(\vec{\sigma})c(\vec{\rho}) \mathrm{e}^{\beta \sum_a \sigma^a \rho^a} + p\gamma \sum_{\vec{\sigma},\vec{\rho},\vec{\tau}} c(\vec{\sigma})c(\vec{\rho})c(\vec{\tau}) \mathrm{e}^{\beta \sum_a \sigma^a \rho^a \tau^a}. \tag{8}$$

In the thermodynamic limit we can calculate the free energy via the saddle point equation obtaining

$$c(\vec{\sigma}) = \exp\left\{ -\Lambda + 2(1-p)\gamma \sum_{\vec{\rho}} c(\vec{\rho}) \exp\left(\beta \sum_a \sigma^a \rho^a\right) + 3p\gamma \sum_{\vec{\rho},\vec{\tau}} c(\vec{\rho})c(\vec{\tau}) \times \exp\left(\beta \sum_a \sigma^a \rho^a \tau^a\right)\right\}. \tag{9}$$

The Lagrange multiplier $\Lambda = -\gamma(2+p)$ ensures the normalization constraint $\sum_{\vec{\sigma}} c(\vec{\sigma}) = 1$ in the limit $n \to 0$. Finding the minimal (zero in the *unfrustrated* case) value of the cost function amounts to studying the $\beta \to \infty$ (zero temperature) properties of the model. In the replica symmetric (RS) ansatz, the behaviour of the spin magnetization can be described in terms of effective fields $m = \tanh \beta h$ whose probability distribution is defined through

$$c(\vec{\sigma}) = \int_{-\infty}^{\infty} \mathrm{d}h\, P(h) \frac{\mathrm{e}^{\beta h \sum_a \sigma^a}}{(2\cosh(\beta h))^n}. \tag{10}$$

In the *unfrustrated* or *ferromagnetic* case, the $P(h)$ turns out to have the simple form

$$P(h) = \sum_{l \geqslant 0} r_l \delta(h-l) \tag{11}$$

where the effective fields only assume integer values. In the *satisfiable* model the saddle point equations all collapse into one single self-consistency equation for r_0:

$$r_0 = \mathrm{e}^{-3p\gamma(1-r_0)^2 - 2(1-p)\gamma(1-r_0)} = \sum_{c_1=0}^{\infty} \sum_{c_2=0}^{\infty} \mathrm{e}^{-3p\gamma} \mathrm{e}^{-2(1-p)\gamma} \frac{(3p\gamma)_1^c}{c_1!} \frac{(2(1-p)\gamma)_2^c}{c_2!} (1-(1-r_0)^2)^{c_1} (r_0)^{c_2}. \tag{12}$$

The equations for the frequency weights r_l with $l > 0$ follow from the one for r_0:

$$r_l = \frac{[3p\gamma(1-r_0)^2 + 2(1-p)\gamma(1-r_0)]^l}{l!}. \tag{13}$$

The previous self-consistency equations for r_0 (or for the magnetization $m = 1 - r_0$) can easily be derived by the same probabilistic argument used in [15], due to the fact that the clause independence allows one to treat the graph and the hyper-graph part separately. Note that in the simple limit $p = 0$ we retrieve the equation for the percolation threshold in a random graph of connectivity γ [19],

$$1 - r_0 = \mathrm{e}^{-2\gamma} \sum_{k=0}^{\infty} \frac{(2\gamma)^k}{k!} (1 - r_0^k). \tag{14}$$

Since the ground state energy of the ferromagnetic model is zero, the free energy coincides with the ground state entropy, which can be written as a function of p, r_0 and γ:

$$S(\gamma) = \log(2)[r_0(1 - \log(r_0)) - \gamma(1-p)(1-(1-r_0)^2) - \gamma p(1-(1-r_0)^3)]. \tag{15}$$

To find the value of the paramagnetic entropy we put ourselves in the phase where all sets of 4- and 2-clauses act independently, each therefore dividing the number of allowed variables

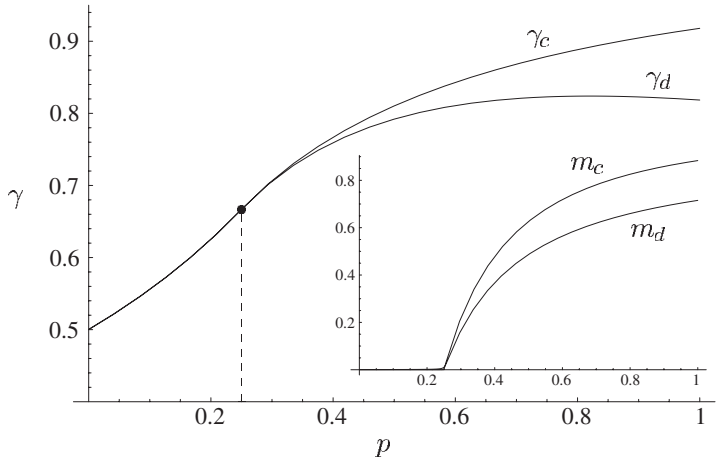

Figure 1. Critical lines (static and dynamic) in the (γ, p) plane. The black dot at (0.667, 0.25) separates continuous transitions from discontinuous ones (where $\gamma_{\rm d} < \gamma_{\rm c}$). Inset: critical magnetizations at $\gamma_{\rm d}(p)$ and $\gamma_{\rm c}(p)$ versus p.

choice by two: the number of ground states will be $N_{\rm gs} = 2^{N-p\gamma N-(1-p)\gamma N} = 2^{N(1-\gamma)}$. The resulting value of $S_{\rm para} = (1-\gamma)\log(2)$ coincides with the one found setting $r_0 = 1$ in equation (15). This may not be the case in more complicated models, where the ground state entropy is a complicated function of γ also for $\gamma < \gamma_{\rm c}$, reflecting the fact that the magnetization probability distribution in the paramagnetic phase could be different from a single delta peak in $m = 0$.

Solving the saddle point equation for r_0, we find that a paramagnetic solution with $r_0 = 1$ always exists, while at a value of $\gamma = \gamma_{\rm d}(p)$ there appears a ferromagnetic solution in the satisfiable model. For $p = 0$, the critical value coincides as expected with the percolation threshold $\gamma_{\rm d}(0) = 1/2$. As long as the model remains like 2-SAT, up to $p < p_0 = 0.25$, the threshold is the point where the ferromagnetic solution appears and also where its entropy exceeds the paramagnetic one. The critical magnetization is zero and the transition is continuous. For larger values of the control parameter p the transition becomes discontinuous. There appears a dynamical transition at $\gamma = \gamma_{\rm d}(p)$ where locally stable solutions appear. At $\gamma = \gamma_{\rm c}(p) > \gamma_{\rm d}(p)$, the non-trivial $r_0 \neq 1$ solution acquires an entropy larger than the paramagnetic one and becomes globally stable. The shape of $\gamma = \gamma_{\rm d}(p)$ and $\gamma = \gamma_{\rm c}(p)$ as functions of p are shown in figure 1. The inset shows the magnetization of the model at the points where the dynamical and the static transitions take place.

4. Numerical simulations

The model can be efficiently solved by a polynomial algorithm based on a representation modulo two (i.e. in Galois field GF[2]). If a formula can be satisfied, then a solution to the following set of M equations in N variables exists:

$$\begin{cases} S_i S_j S_k = T_{ijk} & \forall\{i, j, k\} \in E_3 \\ S_i S_j = J_{ij} & \forall\{i, j\} \in E_2. \end{cases} \tag{16}$$

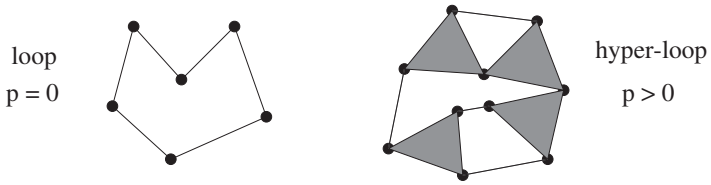

Figure 2. Typical loop and hyper-loop. Lines are 2-spin links, while triangles are 3-spin links. Note that every vertex has an even degree.

Through the mapping $S_i = (-1)^{\sigma_i}$, $J_{ij} = (-1)^{\eta_{ij}}$ and $T_{ijk} = (-1)^{\zeta_{ijk}}$, with $\sigma_i, \eta_{ijk}, \zeta_{ijk} \in \{0, 1\}$, equation (16) can be rewritten as a set of binary linear equations

$$\begin{cases} (\sigma_i + \sigma_j + \sigma_k) \bmod 2 = \zeta_{ijk} & \forall \{i, j, k\} \in E_3 \\ (\sigma_i + \sigma_j) \bmod 2 = \eta_{ij} & \forall \{i, j\} \in E_2. \end{cases} \tag{17}$$

For any given set of couplings $\{\eta_{ij}, \zeta_{ijk}\}$, the solutions to these equations can be easily found in polynomial time by, for example, Gaussian substitution. The solution to the M linear equations in N variables can be summarized as follows: a number $N_{\rm dep}$ of variables is completely determined by the values of the coupling $\{\eta_{ij}, \zeta_{ijk}\}$ and by the values of the $N_{\rm free} = N - N_{\rm dep}$ independent variables. The number of solutions is $2^{N_{\rm free}}$ and the entropy $S(\gamma) = \log(2) N_{\rm free}/N = \log(2)(1 - N_{\rm dep}(\gamma)/N)$. As long as $N_{\rm dep} = M$ we have the paramagnetic entropy $S_{\rm para} = \log(2)(1 - \gamma)$. However, $N_{\rm dep}$ may be less than M when the interactions are such that one can generate linear combinations of equations where no σ appear, like $0 = f(\{\eta_{ij}, \zeta_{ijk}\})$. This kind of equation corresponds to the presence of loops (resp. hyper-loops [15]) in the underlying graph (resp. hyper-graph). A hyper-loop (generalization of a loop on a hyper-graph) is defined as a set $\mathcal{S}$ of (hyper-)links such that every spin (i.e. node) is 'touched' by an even number of (hyper-)links belonging to $\mathcal{S}$ (see figure 2).

Here we are interested in the fraction of satisfiable instances $P_{\rm SAT}(\gamma, p)$, averaged over the random couplings distribution. One can show that, for any random (hyper-)graph, $P_{\rm SAT}$ is given by $2^{-N_{\rm hl}}$, where $N_{\rm hl}$ is the number of independent (hyper-)loops [15]. In figure 3 we show the fraction of satisfiable instances as a function of γ for $p = 0$ and 0.5. The vertical lines report the analytical predictions for the critical points, $\gamma_{\rm c}(p = 0) = 0.5$ and $\gamma(p = 0.5) = 0.810\,343$.

In the limit of large N and for $p = 0.5$ the fraction of SAT instances sharply vanishes at the critical point in a discontinuous way, that is $\lim_{\gamma \to \gamma_{\rm c}^-} P_{\rm SAT}(\gamma) > 0$ while $\lim_{\gamma \to \gamma_{\rm c}^+} P_{\rm SAT}(\gamma) = 0$. This is the usual behaviour already measured in 3-SAT [8, 9] and 3-hyper-SAT [15], with the SAT probabilities measured on finite systems crossing at $\gamma_{\rm c}$ and becoming sharper and sharper as N increases. In contrast, for $p = 0$ and large N the probability of being SAT becomes zero at $\gamma_{\rm c}$ in a continuous way. The main consequence is that finite-size corrections make $P_{\rm SAT}(\gamma)$ larger than its thermodynamical limit both before and after the critical point and thus the data crossing is completely missing.

Note also that for $p < 1$ the fraction of SAT instances for $\gamma < \gamma_{\rm c}(p)$ is finite and less than 1 even in the thermodynamical limit, implying a *mixed phase* of SAT and UNSAT instances. This is due to the presence in the random hyper-graph of loops made only by 2-spin links (indeed the mixed phase is absent for $p = 1$ when only 3-spin interactions are allowed [15]). The expression for the SAT probability in the thermodynamical limit (bold curves in figure 3: the lowermost for $p = 0$ and the uppermost for $p = 0.5$) can be calculated analytically and the final result is

$$P_{\rm SAT}(\gamma, p) = {\rm e}^{\frac{1}{2}\gamma(1-p)[1+\gamma(1-p)]}\,[1 - 2\gamma(1-p)]^{1/4} \qquad \text{for} \quad \gamma \leqslant \gamma_{\rm c}(p). \tag{18}$$

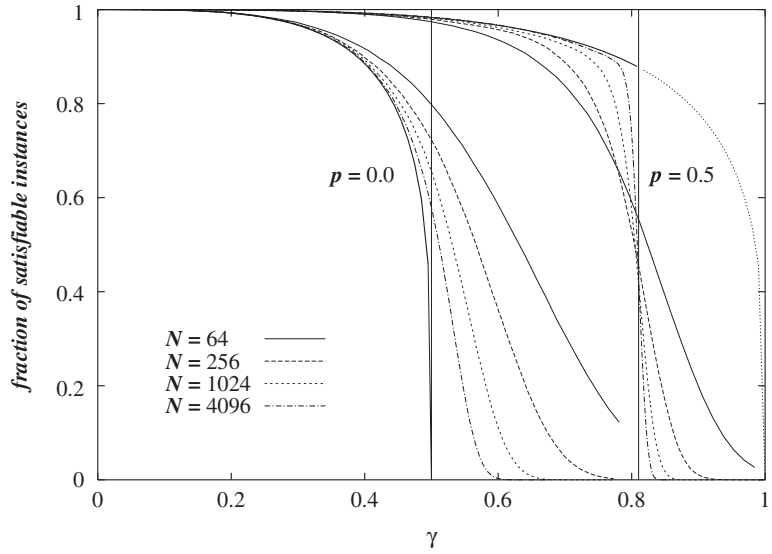

Figure 3. SAT probabilities $P_{\rm SAT}(\gamma, p)$ for $p = 0$ and 0.5. Data have been averaged over 10^4 different random hyper-graphs. Vertical straight lines are analytical predictions for critical points: $\gamma_c(p = 0) = 0.5$ and $\gamma_c(p = 0.5) = 0.810\,343$. Bold curves for $\gamma < \gamma_c$ are analytical predictions for the SAT probability in the large N limit.

In order to obtain to above expression we note that the SAT probability is related to the number of (hyper-)loops by

$$P_{\rm SAT}(\gamma, p) = \sum_{m=0}^{\infty} P(m; \gamma, p) 2^{-m} \tag{19}$$

where $P(m; \gamma, p)$ is the probability of having m (hyper-)loops in a random (hyper-)graph with parameters γ and p, and the factor 2^{-m} comes from the probability that for all the m (hyper-)loops the product of the interactions is 1 (thus giving no contradiction in the formula). In order to estimate $P(m; \gamma, p)$ we may restrict ourselves to considering only simple loops (made of 2-spin links), because hyper-loops which involve at least one 3-spin link are irrelevant in the thermodynamical limit. This can be easily understood with the help of the following counting argument.

The probability that a given 2-spin link is present in a random (γ, p) hyper-graph is $p_2 = 2\gamma(1 - p)/N$ and for a 3-spin hyper-link is $p_3 = 6\gamma p/N^2$. Thus the probability of finding in a random (γ, p) hyper-graph a hyper-loop made of n_2 links and n_3 hyper-links (n_3 must be even) is just the number of different ways one can choose the (hyper-)links times $p_2^{n_2} p_3^{n_3}$. Because the number of nodes belonging to a hyper-loop of this kind is at most $n_n = n_2 + 3n_3/2$ and the number of different hyper-loops of this kind is of order N^{n_n}, we have that the probability of having a hyper-loop with n_2 links and n_3 hyper-links is of order $N^{-n_3/2}$.

Then, for $\gamma < \gamma_c$ the number of hyper-loops is still finite (their number becomes infinite only at γ_c where a transition to a completely UNSAT phase takes place) and the SAT probability, in the large N limit, is completely determined by the number of simple loops ($n_3 = 0$).

The typical number of these loops does not vanish for $\gamma < \frac{1}{2(1-p)}$, and therefore such 'rare' events lead to a coexistence of SAT and UNSAT instances with equal energy density.

The average number of loops of length k can be easily calculated and is given by $x^k/(2k)$, where $x = 2\gamma(1-p)$. The average number of loops of any size

$$A(x) = \sum_{k=3}^{\infty} \frac{x^k}{2k} = -\frac{1}{2}\ln(1-x) - \frac{x}{2} - \frac{x^2}{4} \tag{20}$$

indeed diverges for $x \to 1$, that is for $\gamma \to \frac{1}{2(1-p)}$. The probability of having m loops in a random (γ, p) hyper-graph is then

$$P(m; \gamma, p) = \mathrm{e}^{-A(x)} \frac{A(x)^m}{m!} \tag{21}$$

and the fraction of SAT instances turns out to be the one in equation (18).

We have numerically calculated the SAT probabilities for many p and N values, finding a transition from a mixed to a completely UNSAT phase at the $\gamma_c(p)$ analytically calculated in the previous section. We also find, in agreement with analytical results, that the transition is continuous as long as $p \leqslant 1/4$ and then it becomes discontinuous in the SAT probability.

Let us now concentrate on the scaling with N of the critical region. We have considered several alternative definitions for the critical region. The one we present here seems to be the simplest and also the most robust, in the sense that it can be safely used when the transition is both continuous ($p \leqslant 0.25$) and discontinuous ($p > 0.25$). We assume that the size of the critical region is inversely proportional to the derivative of the SAT probability at the critical point

$$w(N, p)^{-1} = \left.\frac{\partial P_{\mathrm{SAT}}(\gamma, p)}{\partial \gamma}\right|_{\gamma=\gamma_c}. \tag{22}$$

For any value of p the width $w(N)$ goes to zero for large N and the scaling exponent $\nu(p)$ is defined through

$$w(N, p) \propto N^{-1/\nu(p)}. \tag{23}$$

In figure 4 we show, in a log–log scale, $w(N, p)$ as a function of N for many p values, together with the fits to the data. The uppermost and lowermost lines have slopes $-1/3$ and $-1/2$ respectively. Data for $p \leqslant 0.5$ can be perfectly fitted by simple power laws (straight lines in figure 4) and the resulting $\nu(p)$ exponents are reported in figure 5. We note that as long as $p \leqslant 0.25$ the ν exponent turns out to be highly compatible with 3, which is known to be the right value for $p = 0$. Thus we conclude that for $p < 1/4$ the exponents are those of the $p = 0$ fixed point.

For $0.25 < p \leqslant 0.5$ we find that the ν exponent takes non-trivial values between 2 and 3. Then one of the following two conclusions may hold. Either the transition for $p > p_0$ is driven by the $p = 1$ fixed point and the ν exponent is not universal or, more probably, any different p value defines a new universality class. This result is very surprising and interesting for the possibility that different universality classes are simply the consequence of the random hyper-graph topology.

More complicated is the fitting procedure for $p > 0.5$. In a recent paper [14] Wilson has shown that in SAT problems there are intrinsic statistical fluctuations due to the way one construct the formula. This *white noise* induces fluctuations of order $N^{-1/2}$ in the SAT probability. If critical fluctuations decay faster than statistical ones (i.e. $\nu < 2$), in the limit of large N the latter will dominate and the resulting exponent saturates to $\nu = 2$. Data for $p = 0.75$ and 1 shown in figure 4 have a clear upward bending, which we interpret as a crossover from critical (with $\nu < 2$) to statistical ($\nu = 2$) fluctuations. We have fitted these two data sets with a sum of two power laws, $w(N) = AN^{-1/\nu} + BN^{-1/2}$. The goodness of the fits (shown with lines in figure 4) confirm the dominance of statistical fluctuations for large N.

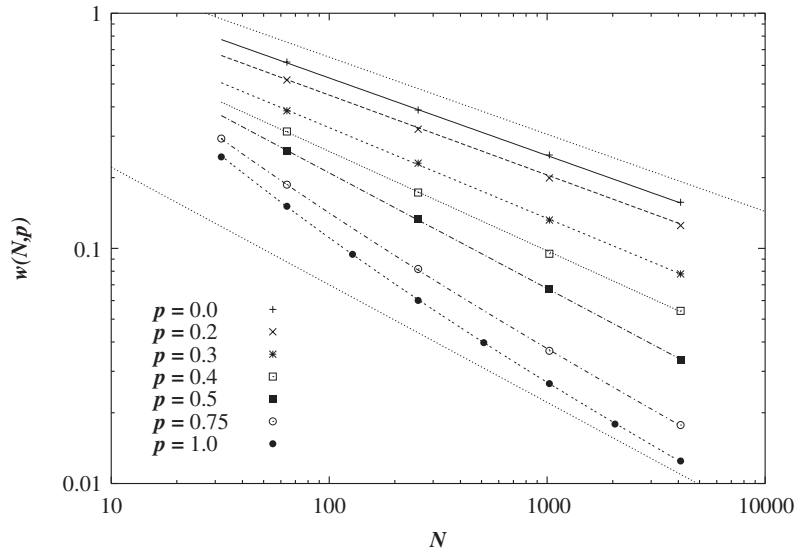

Figure 4. Scaling of the critical window width. Errors are smaller than symbols. Lines are fits to the data.

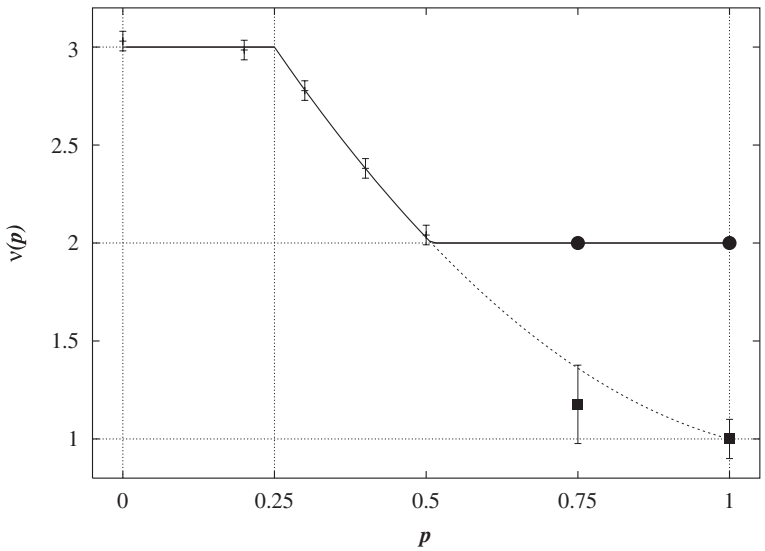

Figure 5. Critical ν exponents obtained from the fits shown in figure 4. For $p = 0.75$ and 1 filled squares show the subleading term power exponent, the leading term one being fixed to $-1/2$ (filled circles).

Moreover, we have also been able to extract a very rough estimate of the critical exponent ν from the subleading term. In figure 5 we show these values with filled squares, and they turn out to be more or less in agreement with a simple extrapolation from $p \leqslant 0.5$ results.

5. Conclusions and perspectives

The exact analysis of a solvable model for the generation of random combinatorial problems has allowed us to show that combinatorial phase diagrams can be affected by rare events leading to a mixed SAT/UNSAT phase. The energy difference between such SAT and UNSAT instances is non-extensive and therefore non-detectable by the usual $\beta \to \infty$ statistical mechanics studies. However, a simple probabilistic argument is sufficient to recover the correct proportion of instances.

Moreover, through the exact location of phase boundaries together with the use of a polynomial global algorithm for determining the existence of solutions we have been able to give a precise characterization of the critical exponents ν depending on the mixing parameter p. The p-dependent behaviour conjectured in [8] for the random $2 + p$ SAT case finds here a quantitative confirmation. The mixing parameter dependency also shows that the value of the scaling exponents is not completely determined by the nature of the phase transition and that the universality class the transition belongs to is very probably determined by the topology of the random hyper-graph. The model we study has also a physical interpretation as a diluted spin glass system. It would be interesting to know whether the parameter-dependent behaviour of critical exponent plays any role in some physically accessible systems.

A last remark on the generalization of the present model: with the same analytical techniques presented here, one can easily solve a Hamiltonian containing a fraction f_k of k-spin interacting terms for any suitable choice of the parameters f_k [20]. The case presented in this paper ($f_2 = 1 - p$ and $f_3 = p$) is the simplest one. There are choices which show a phase diagram still more complex with, for example, a continuous phase transition preceded by a dynamical one.

References

[1] Garey M and Johnson D S 1979 *Computers and Intractability; A Guide to the Theory of NP–Completeness* (San Francisco: Freeman)
Papadimitriou C 1994 *Computational Complexity* (Reading, MA: Addison-Wesley)
[2] Cook S A 1971 *Proc. Third Annual ACM Symp. on Theory of Computing* (New York: ACM) p 151
[3] Hogg T, Huberman B and Williams C (ed) 1996 *Artif. Intell.* **81** Special issue on Phase Transitions and Complexity
[4] Mitchell D, Selman B and Levesque H 1992 *Proc. 10th National Conf. on Artificial Intelligence (AAAI-92)* (Menlo Park, CA: AAAI Press) p 459
[5] Kirkpatrick S and Selman B 1994 *Science* **264** 1297
[6] Goerdt A 1992 *Proc. 17th Int. Symp. on Mathematical Foundations of Computer Science (Lecture Notes in Computer Science vol 629)* (Berlin: Spinger) p 264
Goerdt A 1996 *J. Comput. Syst. Sci.* **53** 469
Chvàtal V and Reed B 1992 *Proc. 33rd IEEE Symp. on Foundations of Computer Science* (New York: IEEE) p 620
[7] Dubois O, Monasson R, Selman B and Zecchina R (ed) 2001 *Theor. Comput. Sci.* Special issue on NP-hardness and Phase Transitions, at press
[8] Monasson R, Zecchina R, Kirkpatrick S, Selman B and Troyansky L 1999 *Nature* **400** 133
[9] Monasson R, Zecchina R, Kirkpatrick S, Selman B and Troyansky L 1999 *Random Struct. Algorithms* **3** 414
[10] Monasson R and Zecchina R 1998 *J. Phys. A: Math. Gen.* **31** 9209
[11] Biroli G, Monasson R and Weigt M 2000 *Eur. Phys. J.* B **14** 551
[12] Monasson R and Zecchina R 1996 *Phys. Rev. Lett.* **76** 3881
Monasson R and Zecchina R 1997 *Phys. Rev.* E **56** 1357
[13] Bollobás B, Borgs C, Chayes J T, Kim J H and Wilson D B 1999 *Preprint* arXiv:math.CO/9909031
[14] Wilson D B 2000 *Preprint* arXiv:math/0005136
[15] Ricci-Tersenghi F, Weigt M and Zecchina R 2001 *Phys. Rev.* E **63** 026702
[16] Creignou N and Daude H 1999 *Discrete Appl. Math.* **96–97** 41
[17] Franz S, Mézard M, Ricci-Tersenghi F, Weigt M and Zecchina R 2001 *Preprint* cond-mat/0103026

[18] Franz S, Leone M, Ricci-Tersenghi F and Zecchina R 2001 *Preprint* cond-mat/0103328
[19] Bollobás B 1985 *Random Graphs* (London: Academic)
[20] Leone M, Ricci-Tersenghi F and Zecchina R in preparation