# New Results on the Phase Transition for Random Quantified Boolean Formulas<sup>\*</sup>

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Abstract. The QSAT problem is the quantified version of the satisfiability problem SAT. We study the phase transition associated with random QSAT instances. We focus on a certain subclass of closed quantified Boolean formulas that can be seen as quantified extended 2-CNF formulas. The evaluation problem for this class is coNP-complete. We carry out an advanced practical and theoretical study, which illuminates the influence of the different parameters used to define random quantified instances.

# 1 Introduction

Recently there has been a growth of interest in a powerful generalization of the Boolean satisfiability, namely the satisfiability of quantified Boolean formulas, QBFs. Compared to the well-known propositional formulas, QBFs permit both universal and existential quantifiers over Boolean variables. Thus QBFs allow for the modeling of problems having higher complexity than SAT, ranging in the polynomial hierarchy up to PSPACE. These problems include problems from the areas of verification, knowledge representation and logic. The numerous applications of QBFs have stimulated the development of practically efficient QBF solvers.

A significant tool for SAT research has been the study of random instances. It has stimulated fruitful interactions among the areas of artificial intelligence, theoretical computer science, mathematics and statistical physics. Encouraged by the widespread embrace of the random SAT model, random instances of QBF have started to attract some attention (see [8,2,11]). Models for generating random instances of QBF have been initiated in [8]. Experimental studies have revealed that QBFs in prenex conjunctive normal form show a sharp transition from satisfiability to unsatisfiability, similar to the one observed for SAT.

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Chen and Interian [2] proposed a mathematically tangible model for generating random instances of QBF. The parameter space of the model offers a richer framework for exploring random instances and their complexity than the SAT model. Our work takes place in this framework. Our goal is to illuminate the role of the different parameters. We focus on particular problems for which we can combine practical experiments with theoretical studies. A first step in this line of research was made in [5], where we studied the QXOR-SAT problem. This problem deals with quantified CNF formulas in which the usual "or" is replaced by the "exclusive or". It has the property of being polynomial time solvable, and thus is a natural candidate to carry out both practical and theoretical studies. Thus, we got new insight on the parameters that influence the nature of the transition from satisfiability to unsatisfiability for XOR-CNF formulas. Here, we continue in this line of research in studying another subclass of formulas, but this time, the evaluation problem is **coNP**-complete. We focus on a certain subclass of closed quantified Boolean formulas that can be seen as quantified extended 2-CNF formulas. This feature provides instances that are still in the reach of the current QBF solvers and also induces some good combinatorial properties that are of use to derive theoretical results.

More precisely, we are interested in closed formulas in conjunctive normal form having two quantifier blocks, namely in formulas of the type  $\forall X \exists Y \varphi(X, Y)$ , where X and Y denote distinct sets of variables, and  $\varphi(X, Y)$  is a conjunction of 3-clauses, each of which contains exactly one universal literal and two existential ones. It is worth noticing that the evaluation problem for this subclass of formulas is **coNP**-complete. Moreover it provides a fixed-length-clause class that smoothly "interpolates" in between P and coNP-complete (see Section 2.1).

In order to generate random instances we have to introduce several parameters. The first one is the pair (m, n) that specifies the number of variables in each quantifier block, i.e., in X and Y. The second one is L = cn, the number of clauses. To sum up the generated formulas are of the form  $\forall X \exists Y \varphi(X, Y)$ , where X has m variables, Y has n variables, each clause in  $\varphi$  has one literal from X and two from Y and there is a total number of cn clauses in  $\varphi$ . We are interested in the probability that a formula drawn at random uniformly out of this set of formulas evaluates to true as n tends to infinity. We will denote by  $\mathbb{P}_{m,c}$  this probability. We are thus interested in

$$\lim_{n \to +\infty} \mathbb{P}_{m,c}(n).$$

We prove that the transition between satisfiability and unsatisfiability for such a random formula occurs when c is in between 1 and 2. Moreover we show that the parameter that controls the location of the transition is m the number of universal variables. For m big enough (as a function of n), there is a *critical* value (or a threshold) of c, c = 1, above which the likelihood of a random formula being satisfiable vanishes as n tends to infinity, and below which it goes to 1. For m small enough, the critical value is at c = 2. An intermediate regime is obtained when m is of logarithmic order compared to n. Our main result is **Theorem 1.** Let  $m = \lceil \alpha \ln n \rceil$  where  $\alpha > 0$ . There exist two decreasing functions a and b with  $1 < a(\alpha) \le b(\alpha) \le 2$  such that the following holds:

$$- if c < a(\alpha), then \mathbb{P}_{m,c}(n) \xrightarrow[n \to +\infty]{} 1,$$
$$- if c > b(\alpha), then \mathbb{P}_{m,c}(n) \xrightarrow[n \to +\infty]{} 0.$$

According to the following partition in three intervals for  $\alpha$  we have:

1. if  $\alpha \leq \frac{1}{\ln 2}$ , then  $a(\alpha) = b(\alpha) = 2$ ,

2. if 
$$\frac{1}{\ln 2} < \alpha \le \frac{2}{\ln 2 - 1/2}$$
, then  $a(\alpha) < b(\alpha) = 2$  and a is strictly decreasing,

3. if  $\alpha > \frac{2}{\ln 2 - 1/2}$ , then  $a(\alpha) < b(\alpha) < 2$ , a and b are strictly decreasing and  $\lim_{\alpha \to +\infty} a(\alpha) = \lim_{\alpha \to +\infty} b(\alpha) = 1$ .

The following figure gives a synthetic picture of the evolution of both lower and upper bounds  $a(\alpha)$ ,  $b(\alpha)$  mentioned in Theorem 1 and explicitly defined in Section 4.



**Fig. 1.**  $a(\alpha)$  and  $b(\alpha)$ 

The paper is organized as follows. First in Section 2 we precisely define the problem we are interested in. We discuss its complexity and finally present the random model. In Section 3, we report some experiments and we show how they have lead to first informations on the phase transition from satisfiability to unsatisfiability. We also illustrate in this section the limits of the experiments. The proof of our main result is inspired by the investigation done by Chvátal, Reed and Goerdt [3,10] in establishing a sharp threshold phenomenon for random 2-SAT (the associated critical ratio being c = 1). It is based on a digraph representation of our formulas presented in Section 4. Then, first and second

moment methods used on specific structures on these graphs give lower and upper bounds for the location of the phase transition. The main steps of the final analytical analysis are given in Section 5.

## 2 Definition of Our Problem

#### 2.1 The Problem (1,2)-QSAT and Its Complexity

A *literal* is a propositional variable or its negation. The *atom* or the propositional variable of a literal l, denoted by |l|, is l itself, if l is of the form p, and p if l is of the form  $\overline{p}$ . A *clause* is a finite disjunction of literals. A formula is in *conjunctive* normal form (CNF) if it is a conjunction of clauses. A formula is in k-CNF, if any clause consists of exactly k literals.

We assume familiarity with the syntax and semantics of quantified Boolean formulas (QBFs). We only consider *closed* QBFs, i.e., QBFs without free variables. A *universal* (*existential*) *literal* is a literal whose atom is universally (existentially) quantified.

Here we are interested in formulas of the form

$$F = \forall X \exists Y \varphi(X, Y)$$

where  $X = \{x_1, \ldots, x_m\}$ , and  $Y = \{y_1, \ldots, y_n\}$ , and  $\varphi(X, Y)$  is a 3-CNF formula, with exactly one universal and two existential literals in each clause. We will call such formulas (1,2)-QCNFs. These formulas can be considered as quantified extended 2-CNF formulas, because deleting the only universal literal in each clause and removing the then superfluous  $\forall$ -quantifiers results in an existentially quantified set of binary clauses. In the following, the 2-CNF formula so obtained will be denoted by  $F_Y = \exists Y \varphi(Y)$ .

A (1,2)-QCNF formula is *true* (or *satisfiable*) if for every assignment to the variables X, there exists an assignment to the variables Y such that  $\varphi$  is true.

Let us give some information about the complexity of the evaluation (true or false) of such formulas. The exhaustive algorithm which consists in deciding whether for all assignment to the variables X, there exists an assignment to the variables Y such that  $\varphi$  is true provides a first upper bound for the worst case complexity. Indeed, since the satisfiability of a 2-CNF formula can be decided in linear time [1], the evaluation of the formula  $\forall X \exists Y \varphi(X, Y)$  can be performed in time  $O(2^m \cdot |\varphi|)$ , where m is the number of universal variables. Observe that if m is bounded by a constant, then it provides a linear time algorithm, and if m is of the order of  $\log n$ , then it provides a polynomial time algorithm. If m has the same order as n, then the above algorithm runs in exponential time. Moreover this problem is in **coNP**: to prove that such a formula is unsatisfiable, guess a vector of truth values  $v_1, \ldots, v_m$  corresponding to  $x_1, \ldots, x_m$ . Replace in  $\exists Y \varphi(X,Y)$  all free occurrences of any  $x_i$  by  $v_i$ , remove  $\perp$  from the clauses and delete clauses with  $\top$ . The resulting formula is a usual 2-CNF formula, whose unsatisfiability can be checked in polynomial time. It is also hard for this class as shown in [7].

### Theorem 2

- For every fixed  $\alpha$ , when restricted to formulas having m universal variables and n existential variables with  $m = \lceil \alpha \ln n \rceil$ , the evaluation problem for (1,2)-QCNF formulas is decidable in polynomial time.
- In its full generality, this evaluation problem is coNP-complete.

It is interesting to note that the same functional dependency between the number of universal variables and the number of existential one, namely  $m = \lceil \alpha \ln n \rceil$ , appears in Theorem 1 and in Theorem 2, thus controlling the location of the transition as well as the complexity of the evaluation problem.

#### 2.2 Random Instances

Let us now describe our model, which is a model suggested in [8] and systematically defined in [2]. The model has several parameters. The first parameter is a pair (m, n) specifying the number of variables in each quantifier block, respectively in X and Y. The second parameter is L, the number of clauses. To sum up the generated formulas are of the form  $\forall X \exists Y \varphi(X, Y)$ , where X has m variables, Y has n variables, each clause in  $\varphi$  has one variable from X and two from Y and there is a total number of L clauses in  $\varphi$ .

Throughout the paper, we reserve m for the number of universal variables, n for the number of existential variables. Note that there are

$$N = m \cdot \binom{n}{2} \cdot 2^3 = 4 \cdot m \cdot n(n-1) \tag{1}$$

clauses. We consider random formulas  $\forall X \exists Y \varphi(X, Y)$  obtained by choosing uniformly independently and with replacement L clauses from all the possible N clauses. We will always consider the parameter m as a function of n, i.e., m = m(n) and L as a fraction of n, i.e., L = cn. Thus, we are interested in the probability that a formula drawn at random uniformly out of this set of formulas is true as n tends to infinity. It is well-known that equivalently, we can consider a formula drawn at random in choosing independently each possible clause with probability p, where  $N \cdot p = c \cdot n$ , that is

$$p \sim \frac{c}{4nm}.$$

We will denote by  $\mathbb{P}_{m,c}(n)$  the probability that such a random formula is true. For fixed n and m,  $\mathbb{P}_{m,c}(n)$  is a decreasing function of c = L/n, which is a control parameter for the transition from satisfiability to unsatisfiability. We will be interested in studying  $\lim_{n \to +\infty} \mathbb{P}_{m,c}(n)$  as a function of the parameters mand c. Any value of c such that  $\mathbb{P}_{m,c}(n) \to 1$  (resp. s. t.  $\mathbb{P}_{m,c}(n) \to 0$ ) gives a lower (resp. upper) bound for the threshold effect associated to the phase transition.

# 3 Experimental Results and a First Estimate for the Location of the Threshold

Before we start discussing the empirical results, let us first describe how we performed the experiments. All experiments have been conducted according to the same scheme, which is described with the help of Fig.2. One experiment consisted in generating at random (in drawing uniformly and independently) (1,2)-QCNF formulas over given values of m universal variables and n existential variables, with a ratio "number of clauses/number of existential variables" varying from 0.85 to 1.2 in steps of 0.05. In Fig. 2, m = n and the values are 5000, 10000, 20000 and 40000. For each of the chosen values of ratio, a sample of 1000 formulas have been studied using the QBF solver QuBE [9], thus computing the truth value of each formula. The proportion of true (or satisfiable) instances for each considered value of ratio has been plotted in Fig. 2.

The experimental results shown in Fig. 2 suggest that, if m = n, then the transition between satisfiability and unsatisfiability occurs when the ratio of number of clauses to number of existential variables, c, is equal to 1. Fig. 3 shows that if m is constant, m = 2, then the transition occurs at c = 2. Moreover, the experiments reported in Fig. 4 indicate that an intermediate regime, with a transition occurring in between 1 and 2, can also be observed.



**Fig. 2.**  $\mathbb{P}_{m,c}$  when m(n) = n. The threshold occurs at c = 1.

These first experiments indicate that the phase transition from satisfiability to unsatisfiability for (1,2)-QCNF formulas occurs when  $1 \le c \le 2$ . The following easy result confirms this observation.

**Proposition 1.** Let m = m(n) be any sequence of integers.

- If c < 1 then  $\mathbb{P}_{m,c}(n) \xrightarrow[n \to \infty]{} 1$ .



**Fig. 3.**  $\mathbb{P}_{m,c}$  when m(n) = 2. The threshold occurs at c = 2.



**Fig. 4.**  $\mathbb{P}_{m,c}$  when m(n) is varying

- If 
$$c > 2$$
 then  $\mathbb{P}_{m,c}(n) \xrightarrow[n \to \infty]{} 0$ .

*Proof.* Let  $F_t$  be the 2-CNF formula obtained from F by setting all the variables  $x_1, \ldots, x_m$  to *true* and omitting all quantifiers. If F is satisfiable, then so is  $F_t$ . Notice that  $F_t$  can be obtained by picking independently each possible 2-clause with probability  $q(n) = 1 - (1 - p(n))^m = \frac{c}{4n} + O(\frac{1}{n^2})$ . Thus the average number of clauses in  $F_t$  is equal to  $4\binom{n(n-1)}{2} \cdot q \sim c/2 \cdot n$ . It follows from the threshold of 2-SAT [3,10] that  $F_t$  is unsatisfiable with probability tending to 1 if c > 2. Thus, the same holds for F. Now, we look at the existential part of the formula,  $F_Y$ . Observe that if  $F_Y$  is satisfiable, then so is F. In  $F_Y$ , each of the  $4\binom{n}{2}$  2-clauses appear independently with probability  $q'(n) = 1 - (1 - p(n))^{2m} = \frac{c}{2n} + O\left(\frac{1}{n^2}\right)$ . Therefore, the threshold of 2-SAT tells us that when c < 1, the formula  $F_Y$  is satisfiable with probability tending to one.

For *m* constant the critical value seems to be at 2, for m = n it seems to be at 1. Then a natural question arises: at what speed should *m* vary so that the critical value is strictly in between 1 and 2? The curves shown in Fig. 4 suggest that a good candidate to look at is when *m* is of logarithmic order compared to *n*. Indeed, each of the curves in this figure corresponds to  $m = \lceil \alpha \ln n \rceil$  for some value  $\alpha$ , respectively for  $\alpha = 9/8$ , 3/2 and 15/8. The following proposition confirms that the logarithmic scale is indeed a good candidate.

**Proposition 2.** Let m = m(n) be a sequence of integers such that  $m \le \ln n / \ln 2$ . If c < 2 then  $\mathbb{P}_{m,c}(n) \xrightarrow[n \to \infty]{} 1$ .

Observe that this result together with Proposition 1 shows a threshold at c = 2 when m is small enough, that is when  $m \leq \ln n / \ln 2$ . In Theorem 1, this corresponds to the first interval, namely  $\alpha \leq \frac{1}{\ln(2)}$ .

To take a step further, a question is whether we can continue to use experiments in order to make precise the critical value when  $m = \lceil \alpha \ln n \rceil$ . Are the solvers, and the machines, powerful enough to provide experiments at a scale big enough?

Figures 5 and 6 show that the critical value of the threshold is very difficult to estimate from the experiments. The experimental results reported in Figure 5 could suggest that all the curves pivot about a single point, thus indicating a critical ratio at  $c \sim 1.8$ . However, as evidenced in Figure 6, which consists



**Fig. 5.**  $\mathbb{P}_{m,c}$  when m(n) = 10. Is the threshold at c = 1.8?



**Fig. 6.**  $\mathbb{P}_{m,c}$  when m(n) = 10. The critical value is difficult to estimate.

in experiments on a finer scale for bigger values of n, one can have successive crossings of pairs of curves for increasing values of n, which provide only a rough estimate of a possible critical ratio. Moreover, the asymptotical behavior (here according to Proposition 2, we have a critical ratio at 2) is still not reached for very big values of n, e.g., for n = 128000.

For this reason, when looking at the case  $m = \lceil \alpha \ln n \rceil$  (for which the complexity is higher than in the case m = 10) one cannot hope that the experiments furnish a reliable estimate on the relationship between the location of the threshold and  $\alpha$ .

# 4 Main Result and Its Relation to 2-SAT

Our main result, which is stated in Theorem 1, shows that the transition occurs for c strictly in between 1 and 2 when the number of universal variables is of a sufficiently large logarithmic order compared to the number of existential variables. Two functions  $a(\alpha)$  and  $b(\alpha)$ , which give respectively a lower and an upper bound for the threshold, are announced in Theorem 1 and shown in Fig. 1. Our probabilistic analysis shows that they are implicitly defined as follows:

 $a(\alpha)$  is the unique solution of  $H(c) = \frac{1}{\alpha}$  for  $c \in ]1, 2[$  where  $H(c) = \ln(c) + \left(\frac{2}{c} - 1\right)\ln(2 - c),$ 

 $b(\alpha)$  is the unique solution of  $K(c) = \frac{1}{\alpha}$  for  $c \in ]1, 2[$  where

$$K(c) = \frac{1}{2} \left( \ln c + \frac{1}{c} - 1 \right).$$

We have  $\lim_{\alpha \to +\infty} a(\alpha) = \lim_{\alpha \to +\infty} b(\alpha) = 1$ . Thus, when  $m/\ln n \xrightarrow[n \to +\infty]{} +\infty$ , Theorem 1 together with Proposition 1 establish a sharp threshold for the satisfiability of (1,2)-QCNF formulas with a critical ratio at c = 1. Since it is easy to derive from [7] that the evaluation problem of (1,2)-QCNF formulas is coNP-complete when restricted to the case m = n, this proves a sharp threshold for a quantified satisfiability problem which is coNP-complete.

In order to prove our main result we will use the relation of our problem to random 2-SAT. Chvátal and Reed introduced specific substructures (bicycles and snakes) on digraphs associated to 2-CNF formulas. Below we will show that their analysis can be adapted to study (1,2)-QCNF random formulas in considering *labeled* digraphs, *pure* bicycles and *simple* snakes. Although the digraph structures associated to 2-CNF and (1,2)-QCNF formulas are very similar, we will need a more involved analysis to describe the probabilistic behavior of *pure* bicycles and *simple* snakes associated to our quantified formulas.

#### 4.1 Representation of (1,2)-QCNF Formulas as Labeled Digraphs

Any (1,2)-QCNF-formula can be represented as a digraph with labeled arcs. For constructing the digraph, we construct the implication digraph [1] associated with the existential 2-CNF formula, and we put the universal literal as a label of the two arcs derived from each clause. Two labels are *dual* if one is x and the other  $\bar{x}$  for some universal variable x. We say that a subgraph of a labeled digraph is *pure* if its set of labels does not contain two dual labels. The maximal pure subgraphs correspond to the implication graphs of the 2-CNF formulas obtained after instantiating the universal variables in the original formula and deleting the quantifiers. Therefore the quantified formula is satisfiable if and only if all the 2-CNF formulas corresponding to the maximal pure subgraphs are satisfiable.

Let  $\phi: \forall x_1 \exists y_1 y_2((x_1 \lor y_1 \lor y_2) \land (\overline{x_1} \lor y_1 \lor \overline{y_2}))$ . The labeled digraph of  $\phi$  is shown on the left in Fig. 7 together with its two maximal pure subgraphs. The first one corresponds to the instantiation  $x_1 = 1$ , whereas the second one corresponds to the instantiation  $x_1 = 0$ .

In order to get lower and upper bounds for the location of the phase transition the idea is to identify specific structures in these graphs that guarantee a formula to be satisfiable (respectively unsatisfiable).

By a bicycle of length  $s+1 \ge 3$ , we mean a set of s+1 clauses  $C_0, \ldots, C_s$  that have the following structure: there are s distinct existential literals  $w_1, \ldots, w_s$ 



**Fig. 7.** The digraph for  $\phi$  together with its maximal pure subgraphs

such that no  $w_i$  is the complement of another, there is a sequence  $v_0, \ldots, v_s$  of s+1 universal literals (or labels), each  $C_r$  with 0 < r < s is  $(v_r \lor \overline{w_r} \lor w_{r+1})$ , and  $C_0 = (v_0 \lor u \lor w_1)$ ,  $C_s = (v_s \lor \overline{w_s} \lor v)$  with literals u, v chosen from  $w_1, \ldots, w_s, \overline{w_1}, \ldots, \overline{w_s}$  with  $(u, v) \neq (w_s, w_1)$ . We consider *pure bicycles*, which are bicycles such that no label is the complement of another.

Claim. Every unsatisfiable (1,2)-QCNF formula contains a pure bicycle.

Let B be the number of pure bicycles in a (1,2)-QCNF formula. In our probabilistic model, we deduce from the above claim and the Markov inequality

$$1 - \mathbb{P}_{m,c}(n) \le \Pr(B \ge 1) \le \mathbb{E}(B).$$
<sup>(2)</sup>

By a snake of length s+1, we mean a set of s+1 clauses  $C_0, \ldots, C_s$ , that have the following structure: there are s distinct existential literals  $w_1, \ldots, w_s$  with s = 2t - 1 such that no  $w_i$  is the complement of another, there is a sequence  $v_0, \ldots, v_s$  of s + 1 universal literals (or labels), each  $C_r$  with  $0 \le r \le s$  is  $(v_r \lor \overline{w_r} \lor w_{r+1})$  with  $w_0 = w_{s+1} = \overline{w_t}$ . We consider simple snakes, which are snakes such that no label is the same as or the complement of another. Note that a simple snake is pure. Simple snakes are easier to enumerate than pure ones and will be sufficient for our purpose. Observe that  $\forall X \exists Y C_0 \land \ldots \land C_s$  is unsatisfiable.

Claim. Every (1,2)-QCNF formula that contains some simple snake is unsatisfiable.

Let X be the number of simple snakes of size s + 1 = 2t in a (1,2)-QCNF formula. In our probabilistic model, we deduce from the above claim and the Cauchy-Schwarz inequality:

$$1 - \mathbb{P}_{m,c}(n) \ge \Pr(X \ge 1) \ge \frac{\left(\mathbb{E}(X)\right)^2}{\mathbb{E}(X^2)}$$
(3)

# 4.2 The First Moment of B and the Second Moment of X

In our probabilistic model, where  $p = \frac{c}{4m(n-1)} \sim \frac{c}{4nm}$ , the following result will be the starting point to get lower bounds for the location of the phase transition.

**Proposition 3.** The mean of the number B of pure bicycles in a random (1,2)-QCNF formula is given by

$$\mathbb{E}(B) = \sum_{s=2}^{n} (n)_s 2^s [(2s)^2 - 1] c(m, s+1) p^{s+1} , \qquad (4)$$

where

$$c(m, s+1) = \sum_{k=1}^{\min(m, s+1)} \binom{m}{k} \cdot 2^k \cdot \mathcal{S}(s+1, k) \cdot k!$$
(5)

with  $\mathcal{S}(m,k)$  denoting the Stirling number of the second kind.

*Proof.* To count B, choose s, the s distinct literals  $w_1, \ldots, w_s$  such that no  $w_i$  is the complement of another, choose u and v, and choose the pure sequence of s + 1 labels  $v_0, \ldots, v_s$  (they are not necessarily distinct but no literal can be the complement of another).

Let c(m, s + 1) be the number of pure sequences of literals of length s + 1, having a set of m variables from which the literals can be built. Let us recall that  $S(m, k) \cdot k!$  is the number of applications from a set of m elements onto a set of k elements. A pure sequence of literals of length s + 1 is obtained by exactly one sequence of choices of the following choosing process.

- 1. Choose the number k of different variables occurring in the sequence.
- 2. Choose the k variables
- 3. For each such variable, choose whether it occurs positively or negatively.
- 4. Choose their places in the sequence.

As in [3], the following observation will be the starting point to get upper bounds for the location of the phase transition:

**Proposition 4.** Let X be the number of simple snakes of size s + 1 = 2t in a (1,2)-QCNF formula. Then

$$\frac{(\mathbb{E}(X))^2}{\mathbb{E}(X^2)} = \frac{1}{q_0(m,n) + \sum_{i=1}^{2t} q_i(m,n) \cdot p^{-i}}$$
(6)

where

$$q_i(m,n) = \frac{\#\{simple \ snakes \ B \ such \ that \ |A_0 \cap B| = i\}}{\#\{simple \ snakes\}}$$
(7)

for any fixed simple snake  $A_0$ , with  $|A_0 \cap B|$  denoting the number of clauses  $A_0$ and B share.

### 5 Proofs

#### 5.1 Proof of Proposition 2

Coming back to the first moment of B, we get from equation (4):

$$\mathbb{E}(B) \le \frac{c}{nm} \sum_{s=2}^{n} s^2 (\frac{c}{2m})^s c(m, s+1) .$$
(8)

Notice that c(m, s+1) is bounded from above by  $2^{\min\{m, s+1\}}$  times the number of applications from  $\{1, \ldots, s+1\}$  to  $\{1, \ldots, m\}$ :

$$c(m, s+1) \le 2^{\min\{m, s+1\}} m^{s+1}$$
 (9)

When  $x \in [0, 1[$  and  $r \ge 1$ , standard computations show that:

$$\sum_{s=r}^{\infty} s^2 x^s \le r^2 \frac{x^r}{(1-x)^3} \,. \tag{10}$$

Thus, when 1 < c < 2, then  $\mathbb{E}(B) \le \frac{c}{n} \sum_{s=2}^{m-1} s^2 c^s + \frac{c2^m}{n} \sum_{s=m}^{\infty} s^2 \left(\frac{c}{2}\right)^s = O\left(m^2 \frac{c^m}{n}\right)$ , which goes to zero as n goes to infinity when  $m \le \ln n / \ln 2$ . Proposition 2 is proved.

# 5.2 Proof of the Lower Bound in Theorem 1

By using precise results for the behavior of Stirling numbers of the second kind [12] (already used in [6] and [5]), a finer analysis of the expected number of pure bicycles as expressed in (4) gives the following result.

**Theorem 3.** When 1 < c < 2, and  $m = \lceil \alpha \ln n \rceil$  with  $\alpha > \frac{1}{\ln(2)}$ , the average number of pure bicycles satisfies

$$\mathbb{E}(B) \le C(\ln n)^{9/2} \cdot n^{\alpha H(c) - 1} + o(1),$$

where C is a constant depending only on  $\alpha$  and c, and  $H(c) = \ln(c) + \left(\frac{2}{c} - 1\right)\ln(2-c)$ .

Let  $a(\alpha)$  be the solution of the equation  $\alpha \cdot H(c) = 1$ , then for  $c < a(\alpha)$  the above result shows that  $\mathbb{E}(B) = o(1)$ . Thus, with (2) we deduce the lower bound stated in Theorem 1.

# 5.3 Proof of the Upper Bound in Theorem 1

When considering simple snakes and making a similar estimation as in equations (8) and (9) in [3], we get the following result.

**Theorem 4.** When 1 < c < 2,  $m = \lceil \alpha \ln n \rceil$  and for  $t = \lceil \frac{\alpha}{2}(1 - \frac{1}{c}) \ln(n) \rceil$  we have

$$\sum_{i=1}^{2t} q_i(m,n) p^{-i} = O\left(\max\left(\ln(n) \cdot n^{1-\alpha K(c)}, \frac{(\ln n)^{10}}{n}\right)\right)$$
  
where  $K(c) = \frac{1}{2} \left(\ln c + \frac{1}{c} - 1\right)$ .

Let  $b(\alpha)$  be the solution of the equation  $\alpha \cdot K(c) = 1$  then  $b(\alpha) < 2$  when  $\alpha > \frac{2}{\ln(2) - 1/2}$ . For  $c > b(\alpha)$  the above result shows that  $\sum_{i=1}^{2t} q_i(m, n)p^{-i} = o(1)$ . Observe that  $\sum_{i=0}^{2t} q_i(m, n) = 1$ , then with (3) and (6) we get the upper bound stated in Theorem 1.

## 6 Conclusion

We have made an extensive study of a natural and expressive quantified problem. The obtained results have several interesting features. They highlight the role of different parameters and their influence on the transition. These results are based on experiments that make use of a current QBF solver. These experiments are carried out at a scale large enough in order to give a useful intuition on the asymptotical behavior of random instances. We have shown that functional dependencies other than  $m = \rho n$  can be important. Indeed, we have demonstrated that  $m = \lceil \alpha \ln n \rceil$  is the scale which is crucial, both for the complexity and the behavior of random instances (see Theorems 1 and 2). Moreover, we give the precise location of the sharp phase transition (namely at c = 1) for a natural quantified problem (namely when m = n) which is coNP-complete.

# References

- Aspvall, B., Plass, M.F., Tarjan, R.E.: A linear-time algorithm for testing the truth of certain quantified Boolean formulas. Information Processing Letters 8(3), 121– 123 (1979)
- Chen, H., Interian, Y.: A model for generating random quantified Boolean formulas. In: Proceedings of the 19th International joint Conference on Artificial Intelligence, IJCAI 2005, pp. 66–71 (2005)
- Chvátal, V., Reed, B.: Mick gets some (the odds are on his side). In: Proceedings of the 33rd Annual Symposium on Foundations of Computer Science, FOCS 1992, pp. 620–627 (1992)
- Creignou, N., Daudé, H., Dubois, O.: Expected number of locally maximal solutions for random Boolean CSPs. In: Proceedings of the13th International Conference on Analysis of Algorithms, AofA 2007, Antibes, June 2007. DMTCS, pp. 507–516 (2007)
- Creignou, N., Daudé, H., Egly, U.: Phase transition for random quantified XORformulas. Journal of Artificial Intelligence Research 19, 1–18 (2007)
- Dubois, O., Boufkhad, Y.: A general upper bound for the satisfiability threshold of random r-SAT formulae. Journal of Algorithms 24(2), 395–420 (1997)
- Flögel, A., Karpinski, M., Kleine Büning, H.: Subclasses of quantified Boolean formulas. In: Schönfeld, W., Börger, E., Kleine Büning, H., Richter, M.M. (eds.) CSL 1990. LNCS, vol. 533, pp. 145–155. Springer, Heidelberg (1991)
- 8. Gent, I.P., Walsh, T.: Beyond NP: the QSAT phase transition. In: Proceedings of AAAI 1999 (1999)
- Giunchiglia, E., Narizzano, M., Tacchella, A.: QuBE: A System for Deciding Quantified Boolean Formulas Satisfiability. In: Goré, R.P., Leitsch, A., Nipkow, T. (eds.) IJCAR 2001. LNCS (LNAI), vol. 2083, pp. 364–369. Springer, Heidelberg (2001)
- Goerdt, A.: A threshold for unsatisfiability. Journal of of Computer and System Sciences 53(3), 469–486 (1996)
- Interian, Y., Corvera, G., Selman, B., Williams, R.: Finding small unsatisfiable cores to prove unsatisfiability of QBFs. In: Proceedings of the 9th International Symposium on Artificial Intelligence and Mathematics (2006)
- Temme, N.M.: Asymptotic estimates of Stirling numbers. Stud. appl. Math. 89, 223–243 (1993)