

## Guarded negation

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We consider restrictions of first-order logic and of fixpoint logic in which all occurrences of negation are required to be guarded by an atomic predicate. In terms of expressive power, the logics in question, called GNFO and GNFP, extend the guarded fragment of first-order logic and the guarded least fixpoint logic, respectively. They also extend the recently introduced unary negation fragments of first-order logic and of least fixpoint logic.

We show that the satisfiability problem for GNFO and for GNFP is 2ExpTime-complete, both on arbitrary structures and on finite structures. We also study the complexity of the associated model checking problems. Finally, we show that GNFO and GNFP are not only computationally well behaved, but also model theoretically: we show that GNFO and GNFP have the tree-like model property and that GNFO has the finite model property, and we characterize the expressive power of GNFO in terms of invariance for an appropriate notion of bisimulation.

Our complexity upper bounds for GNFO and GNFP hold true even for their “clique-guarded” extensions CGNFO and CGNFP, in which clique guards are allowed in the place of guards.

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## 1. INTRODUCTION

Modal logic is well known for its “robust decidability”: not only are basic decision problems such as satisfiability, validity and entailment decidable, but the decidability of these problems is preserved under various natural variations and extensions to the syntax and semantics of modal logic (e.g., addition of fixpoint operators, backward modalities, nominals; restriction to finite structures). As observed by Vardi [Vardi 1996], this robust decidability is intimately linked to the fact that modal logic has a combination of three properties, namely (i) the *tree model property* (if a formula has a model, it has a model which is a tree), (ii) *translatability into tree automata* (each formula can be transformed into a tree automaton, or equivalently, an MSO formula, recognizing its tree models) and, (iii) the *finite model property* (every satisfiable modal formula is satisfied in a finite structure). The decidability of satisfiability for modal logic, both on arbitrary structures and on finite structures, follows immediately from these three properties. Similar arguments can be used to show the good behavior of many extensions of modal logic, although we should note here that the two-way

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$\mu$ -calculus (the extension of modal logic with fixpoint operators and backward modalities) lacks the finite model property, and hence the decidability of satisfiability on finite structures for this logic involves a separate (non-trivial) argument [Bojańczyk 2003].

The properties (i), (ii) and (iii) described above can be viewed as a semantic explanation for the robust decidability of modal logic. Given that modal logic can be viewed as a syntactic fragment of first-order logic, it is also natural to ask for syntactic explanations: *what syntactic features of modal formulas (viewed as first-order formulas) are responsible for their good behavior? And can we generalize modal logic, preserving these features, while at the same time dropping inessential restrictions inherent in modal logic (such as the fact that it can only describe structures with unary and binary relations)?*

Several answers to these questions have been proposed. The first one is to consider the two variable fragment of first-order logic, which is decidable and has the finite model property [Mortimer 1975]. Unfortunately, this observation does not go very far towards explaining the robust decidability of modal logic, since it seems impossible to extend the two variable fragment with a fixpoint mechanism while maintaining decidability [Grädel et al. 1999].

The second proposal is to consider logics with guarded quantifications. The *guarded fragment* of first-order logic (GFO), introduced in [Andréka et al. 1998], consists of FO formulas in which all quantifiers are “guarded” by atomic predicates. It has a natural extension with fixpoint operators (GFP) that extends the two-way  $\mu$ -calculus [Grädel and Walukiewicz 1999]. Both GFO and GFP have the tree-like model property (if a formula has a model, it has one of bounded tree width), they can be translated into tree automata (each formula can be transformed into a tree automaton recognizing tree decompositions of its models of bounded tree width) and GFO has the finite model property [Andréka et al. 1998; Grädel 2001]. Finite satisfiability of GFP was only recently proved decidable in [Bárány and Bojańczyk 2012].

The third, and most recent proposal is based on unary negation. Unary negation first-order logic (UNFO) restricts first-order logic by constraining the use of negation to subformulas having at most one free variable (and viewing universal quantification as a defined connective). Unary negation fixpoint (UNFP) is the natural extension of UNFO using monadic fixpoints. Again, UNFO generalizes modal logic, and UNFP generalizes the two-way  $\mu$ -calculus. Both UNFO and UNFP have the tree-like model property, they can be translated into tree automata and UNFO has the finite model property [ten Cate and Segoufin 2013]. Decidability of finite satisfiability for UNFP was also established in [ten Cate and Segoufin 2013].

The three extensions of modal logics presented above are incomparable in terms of expressive power. In particular there are properties expressible in UNFO that are not expressible in GFO and vice-versa. In this paper we unify the unary negation and guarded quantification approaches by introducing guarded-negation logics.

*Guarded-negation first-order logic* (GNFO) restricts FO by requiring that all occurrences of negation are of the form  $\alpha \wedge \neg \phi$  where the “guard”  $\alpha$  is an atomic formula (possibly an equality statement) containing all the free variables of  $\phi$ . For instance, GNFO cannot express  $x \neq y$  but it can express  $R(x, y, z) \wedge x \neq y$ . We also disallow universal quantification as a primitive connective (though a limited form of universal quantification can be expressed using existential quantification and guarded negation). For instance, GNFO cannot express  $\forall \bar{x} R(\bar{x})$  but it can express  $\forall \bar{x} S(\bar{x}) \rightarrow R(\bar{x})$  as  $\exists y y = y \wedge \neg(\exists \bar{x} S(\bar{x}) \wedge \neg R(\bar{x}))$ . Guarded-negation fixpoint logic (GNFP) extends GNFO with a guarded fixpoint mechanism. In terms of expressive power, GNFO forms a strict extension of both UNFO and GFO.

We show that our guarded-negation logics have the same desirable properties as modal logics, unary negation logics and guarded logics: Both GNFO and GNFP have the tree-like model property, they can be translated into tree automata and GNFO has the finite model property.

More precisely, we show that the satisfiability problem for GNFO and GNFP is decidable, both on arbitrary structures and on finite structures. These two problems are both 2ExpTime-complete,

even for a fixed finite signature (in contrast the satisfiability of GFO decreases from 2ExpTime to ExpTime when the signature is fixed).

We also study the (combined) complexity of the model checking problem of GNFO and GNFP. The problem is  $P^{NP^{O(\log^2 n)}}$ -complete for GNFO. In the case of GNFP, it is hard for  $P^{NP}$  and contained in  $NP^{NP} \cap coNP^{NP}$ . These results are obtained using a simple polynomial time reduction to their unary negation variants, UNFO and UNFP, whose model checking was solved in [ten Cate and Segoufin 2013]. Recall that the model checking problem of GFO is PTime-complete [Berwanger and Grädel 2001] and that a similar gap between the upper bound and the lower bound exists for GFP and the  $\mu$ -calculus, where the complexity of model checking is known to lie between PTime and  $NP \cap coNP$  [Berwanger and Grädel 2001].

Next, we explore the model theory of GNFO. We define a guarded-negation variant of bisimulation suitable for guarded-negation logics and most of our results build on the fact that guarded-negation logics are invariant under guarded-negation bisimulations. The appropriateness of guarded-negation bisimulation is illustrated by showing that GFO is exactly the fragment of first-order logic that is invariant under guarded-negation bisimulation.

Finally, we show that our complexity results can be lifted to the *clique-guarded* extensions of GNFO and GNFP, which provide a further generalization of GNFO and GNFP that subsume the *clique-guarded fragment* (as well as the closely related *loosely guarded fragment* and *packed fragment*) [van Benthem 1997; Marx 1999; Grädel 1999a].

The most involved result is the decidability of satisfiability on finite structures. For GNFO, we give a reduction to testing whether a union of conjunctive queries is implied by a guarded formula, recently shown decidable in [Bárány et al. 2014]. In the case of GNFP, we make a reduction to the decidability of finite satisfiability of GFP, recently proved in [Bárány and Bojańczyk 2012].

An extended abstract of this paper was published in [Bárány et al. 2011]. The present paper provides detailed proofs of the results presented there. In particular we have clarified and fixed several issues concerning certain definitions. In addition, it contains new material concerning syntactic variants of guarded-negation fixpoint logic, and concerning clique-guarded negation logics.

*Outline of the paper.* Guarded-negation first-order logic, GNFO, is presented in Section 2 and its satisfiability is shown decidable in Section 3. The fixpoint extension of GNFO, GNFP, is introduced in Section 4 where it is shown to be decidable via a reduction to GFP. The same reduction also implies the finite model property of GNFO. The model checking problems of GNFO and GNFP are studied in Section 5. A variant of bisimulation suitable for guarded-negation formulas is introduced in Section 6, where it is also shown that GNFO is exactly those first-order formulas closed under guarded-negation bisimulation. The tree-like model property of GNFO and GNFP is derived from this notion. Finally, in Section 7, we extend our results to a generalization of GNFO and GNFP with clique-guards.

## 2. PRELIMINARIES

**Structures and formulas.** We restrict our attention to relational structures. However, as we will explain in Section 7.2, all complexity results presented in this paper generalize to the case with constant symbols.

A (relational) *signature*  $\tau$  is a finite set of relation symbols, each having an associated arity. By the *arity of a signature*, we mean the maximal arity of its relations. A *structure*  $M$  over a relational signature  $\tau$  consists of a set  $dom(M)$ , the *domain* of  $M$ , together with an interpretation  $R^M$  of each relation symbol  $R \in \tau$ , which is a  $k$ -ary relation over  $dom(M)$ , where  $k$  is the arity of  $R$  according to  $\tau$ . A structure  $M$  is said to be *finite* if  $dom(M)$  is finite. An *expansion* of a structure  $M$  over  $\tau$  is a structure  $M'$  over a signature  $\sigma \supseteq \tau$  such that  $M$  and  $M'$  agree on their domain and on the interpretation of all relation symbols in  $\tau$ . If a tuple of elements  $\bar{a}$  from  $dom(M)$  belongs to the interpretation of a relation symbol  $R$ , then we say that  $R(\bar{a})$  is a *fact* of  $M$ . A set of elements of  $M$  is *guarded* (in  $M$ ) if it is either a singleton set or there is a fact of  $M$  containing all its elements.

A tuple of elements of  $M$  is guarded if the set of elements occurring in the tuple is guarded. We denote by  $\text{guarded}(M)$  the set of all guarded tuples of  $M$ . If  $M$  and  $N$  are structures and  $\bar{a}$  and  $\bar{b}$  are tuples of elements from  $\text{dom}(M)$  and  $\text{dom}(N)$ , respectively, then we say that  $(M, \bar{a})$  and  $(N, \bar{b})$  are *locally isomorphic* if there is a partial isomorphism  $f : M \rightarrow N$  such that  $f(\bar{a}) = \bar{b}$ .

We assume familiarity with first-order logic, FO, and least fixpoint logic, LFP, over relational structures. We use classical syntax and semantics for FO and LFP. The *size of a formula*  $\phi$ , denoted by  $|\phi|$ , is the number of symbols needed to write down the formula. We use the notation  $\phi(\bar{x})$  to indicate that the free variables of  $\phi$  are exactly the variables in  $\bar{x}$ . A *sentence* is a formula with no free variable. We say that a structure  $M$  is a *model* of a sentence  $\phi$  if  $M \models \phi$ . We also write  $M \models \phi(\bar{u})$  or  $(M, \bar{u}) \models \phi(\bar{x})$  when a tuple  $\bar{u}$  of elements of the structure  $M$  makes the formula  $\phi(\bar{x})$  true in  $M$ . Finally we write  $\models \varphi$  if  $\varphi$  is true in all structures.

**Conjunctive queries.** A conjunctive query (CQ) is a first-order formula of the form

$$\exists y_1 \cdots y_l (\alpha_1 \wedge \alpha_2 \wedge \dots \wedge \alpha_n)$$

where each  $\alpha_i$  is an atomic formula, possibly an equality statement. A union of conjunctive queries (UCQ) is a disjunction of CQs. A positive-existential query is a first-order formula built using disjunction, conjunction and existential quantification only. Every positive-existential query can be transformed in a UCQ at the cost of a possible exponential blow-up. The *width* of a CQ is the number of variables occurring in it, and the width of a UCQ is the maximum width of its CQs. The *height* of a UCQ is the maximum size of its CQs. In particular the height of a CQ is its size.

**GNFO.** We define GNFO, *guarded-negation first-order logic*, as the fragment of FO given by the following grammar, where  $R$  ranges over predicate symbols, and  $\alpha(\bar{x}\bar{y})$  is an atomic formula (possibly an equality statement).

$$\varphi ::= R(\bar{x}) \mid x = y \mid \exists x \varphi \mid \varphi \vee \varphi \mid \varphi \wedge \varphi \mid \alpha(\bar{x}\bar{y}) \wedge \neg\varphi(\bar{y}) \quad (1)$$

Hence the logic can only negate a subformula if all its free variables are “guarded” by some fact, or if the subformula has at most one free variable (in which case one can use an equality statement of the form  $x = x$  or  $y = y$  as the guard). For example,  $x \neq y$  is not a formula of GNFO but  $R(x, y, z) \wedge x \neq y$  is. Notice that all positive-existential queries belong to GNFO. We write  $\text{GNFO}[\tau]$  for the set of formulas using relation symbols in the signature  $\tau$ .

We will refer to formulas of the form  $\alpha(\bar{x}\bar{y}) \wedge \varphi'(\bar{x})$  (where  $\alpha$  is an atomic formula) as *answer-guarded formulas*. In addition, we consider every atomic formula by itself to be an answer-guarded formula (motivated by the fact that  $\alpha(\bar{x})$  is equivalent to  $\alpha(\bar{x}) \wedge \alpha(\bar{x})$ ).

We say that a formula of GNFO is in *GN-normal form* if, in its syntax tree, no disjunction is directly below an existential quantifier or a conjunction, and no existential quantifier is directly below a conjunction sign. Every GNFO formula can be brought into GN-normal form, at the cost of an exponential increase in length and linear increase in the number of variables, by pushing out disjunction and pushing in conjunctions using the following rewriting rules (where  $x'$  is a variable not occurring in  $\psi \wedge \phi$  and  $\phi[x'/x]$  is the formula constructed from  $\phi$  by replacing all occurrences of  $x$  by  $x'$ ):

$$\begin{aligned} \exists x (\phi \vee \psi) &\rightarrow \exists x \phi \vee \exists x \psi \\ \phi \wedge (\psi \vee \chi) &\rightarrow (\phi \wedge \psi) \vee (\phi \wedge \chi) \\ (\exists x \phi) \wedge \psi &\rightarrow \exists x' (\phi[x'/x] \wedge \psi) \end{aligned}$$

The appeal of the GN-normal form is that it highlights the fact that GNFO formulas can be naturally viewed as being built up from atomic formulas using guarded negation, and unions of conjunctive queries. Indeed, the GNFO formulas in GN-normal form are precisely generated by the following recursive definition:

$$\varphi ::= R(\bar{x}) \mid x = y \mid \alpha(\bar{x}\bar{y}) \wedge \neg\varphi(\bar{y}) \mid q[\varphi_1/U_1, \dots, \varphi_s/U_s] \quad (2)$$

where  $q$  is a UCQ using relation symbols  $U_1, \dots, U_s$ , and  $\varphi_1, \dots, \varphi_s$  are answer-guarded formulas generated by the same recursive definition with the appropriate number of free variables corresponding to the relation symbols they replace. Here,  $q[\varphi_1/U_1, \dots, \varphi_s/U_s]$  is the result of replacing in  $q$  all subformulas of the form  $U_i(\bar{x})$  with  $i \leq s$  by  $\varphi_i(\bar{x})$ .

A formula of GNFO is said to be *of width  $k$*  if, when brought into GN-normal form in the way described above, it uses at most  $k$  variables (or equivalently, is built up using UCQs  $q$  of width at most  $k$ ). We denote by  $\text{GNFO}^k$  all GNFO formulas of width  $k$ .

*Example 2.1.* Consider for example the existential positive formula

$$\exists xy (R(x) \wedge \exists z T(x, y, z) \wedge \exists z' S(x, z')).$$

When brought into GN-normal form it gives

$$\exists xyz z' R(x) \wedge T(x, y, z) \wedge S(x, z').$$

and has width 4. Notice that it is also equivalent to the GNFO formula

$$\exists xyz R(x) \wedge T(x, y, z) \wedge \neg\neg(\exists z S(x, z))$$

that is in GN-normal form and has width 3. Recall that  $\neg\neg(\exists z S(x, z))$  is indeed a formula of GNFO as it negates unary formula and those could be seen as guarded by an equality atom. In other words it is equivalent to  $x = x \wedge \neg(x = x \wedge \neg(\exists z S(x, z)))$

**GNFO extends GFO and UNFO.** GNFO generalizes the unary negation logic, UNFO, studied in [ten Cate and Segoufin 2013], which only allows the negation of formulas having at most one free variable. It also generalizes the *guarded fragment of first-order logic* (GFO). The logic GFO is the fragment of FO defined by the following grammar, where, again,  $\alpha(\bar{x}\bar{y}\bar{z})$  is an atomic formula (possibly an equality statement):

$$\varphi ::= R(\bar{x}) \mid x = y \mid \varphi \vee \varphi \mid \varphi \wedge \varphi \mid \neg\varphi \mid \exists \bar{x} \alpha(\bar{x}\bar{y}\bar{z}) \wedge \varphi(\bar{x}\bar{y}) \mid \forall \bar{x} \alpha(\bar{x}\bar{y}\bar{z}) \rightarrow \varphi(\bar{x}\bar{y})$$

It is straightforward to check that:

**PROPOSITION 2.2.** *Every GFO sentence is equivalent to a GNFO sentence, via a polynomial time transformation.*

This result extends to answer-guarded formulas, however  $\neg R(xy)$  is in GFO but not expressible in GNFO.

**PROOF.** Consider a GFO-sentence  $\varphi$ . Because  $\varphi$  is closed, every subformula  $\vartheta(\bar{x})$  of  $\varphi$  with free variables  $\bar{x}$  falls in the scope of an (innermost) guarded quantifier with some guard, let us refer to it as  $\alpha_{\vartheta}(\bar{x}\bar{u})$ . We can therefore safely replace in  $\varphi$  each negated subformula  $\vartheta(\bar{x})$  of the form  $\neg\psi(\bar{x})$  with  $(\alpha_{\vartheta}(\bar{x}\bar{u}) \wedge \vartheta(\bar{x}))$ . Each universally quantified subformula  $\vartheta(\bar{x}\bar{z})$  of the form  $\forall \bar{y} \alpha(\bar{x}\bar{y}\bar{z}) \rightarrow \psi(\bar{x}\bar{y})$  is equivalent to  $\neg\exists \bar{y} (\alpha(\bar{x}\bar{y}\bar{z}) \wedge \neg\psi(\bar{x}\bar{y}))$ . It can therefore be replaced in  $\varphi$  by  $\alpha_{\vartheta}(\bar{x}\bar{z}\bar{u}) \wedge \neg(\exists \bar{y} \alpha(\bar{x}\bar{y}\bar{z}) \wedge \neg\psi(\bar{x}\bar{y}))$ . Let  $\hat{\varphi}$  be the sentence so obtained from  $\varphi$ . By construction,  $\hat{\varphi}$  is a sentence of GNFO, and it is easy to see that  $\hat{\varphi}$  is logically equivalent to  $\varphi$ .  $\square$

The following example shows that GNFO is strictly more expressive than GFO and UNFO.

*Example 2.3.* The GNFO sentence  $\delta$  defined as

$$\exists xy (E(x, y) \wedge \neg\exists uvw (E(x, u) \wedge E(u, v) \wedge E(v, w) \wedge E(w, y)))$$

is not equivalent to any GFO sentence or to any UNFO sentence, even on undirected graphs. This is because  $\delta$  defines a property that is not invariant under guarded bisimulation (which, incidentally, amounts to ordinary bisimulation in case of simple graphs), as can be easily verified, nor is it invariant under ‘‘UN-bisimulation’’ as befits UNFO formulas, cf. [ten Cate and Segoufin 2013].

### 3. THE SATISFIABILITY PROBLEM FOR GNFO

In this section we show that (finite) satisfiability for GNFO is 2EXPTIME-complete. The 2EXPTIME lower bound follows immediately from the fact that satisfiability for UNFO is already hard for 2EXPTIME [ten Cate and Segoufin 2013; Grädel 1999b]. It holds even if the signature is fixed (recall that when the signature is fixed the complexity of satisfiability for GFO is ExpTime-complete).

The upper bound is proved using a reduction to the problem of testing whether a GFO formula entails (on finite structures) a UCQ. The latter problem is also known as the problem of query answering against a GFO theory, and it has been solved in [Bárány et al. 2014]. To streamline the presentation, we will allow the possibility of zero-ary relation symbols.

The reduction is obtained by rewriting the formula by adding new relational symbols in order to simplify it while preserving its satisfiability status. The first step is the following lemma.

**LEMMA 3.1.** *Given any formula  $\varphi(\bar{x}) \in \text{GNFO}[\tau]$  we can construct in polynomial time a companion formula  $\psi(\bar{x}) \in \text{GNFO}[\tau \cup \sigma]$  of the form*

$$\psi(\bar{x}) = \underbrace{S(\bar{x}) \wedge \bigwedge_j \forall \bar{z}\bar{u} R_j(\bar{z}\bar{u}) \rightarrow q_j(\bar{z})}_{\psi^+} \wedge \underbrace{\bigwedge_i \forall \bar{z}\bar{u} T_i(\bar{z}\bar{u}) \rightarrow \neg p_i(\bar{z})}_{\psi^-} \quad (3)$$

where  $\sigma$  is the signature (disjoint from  $\tau$ ) consisting of the relation symbols  $S$  and  $T_i$ <sup>1</sup>, where the  $R_j$  are atomic formulas, the  $q_j$ 's and  $p_i$ 's are positive-existential first-order formulas,  $\text{width}(\psi) = \text{width}(\varphi)$  and such that

$$\models \varphi \leftrightarrow \exists \sigma \psi$$

where  $\exists \sigma$  is a shorthand for the existential second-order quantification of all the symbols in  $\sigma$ .

**PROOF.** Given a GNFO-formula  $\varphi$  consider an inner-most occurrence of a guarded negation  $R(\bar{z}\bar{u}) \wedge \neg q(\bar{z})$  as a subformula of  $\varphi$ . Then  $q(\bar{z})$  is necessarily positive existential. Let  $T$  be a new predicate symbol of the same arity as  $R$ . We substitute  $T(\bar{z}\bar{u})$  in the input formula for the subformula  $R(\bar{z}\bar{u}) \wedge \neg q(\bar{z})$ , and add the following as conjuncts to  $\psi^+$  and  $\psi^-$ , according to their kind.

$$\begin{aligned} \forall \bar{z}\bar{u} T(\bar{z}\bar{u}) &\rightarrow \neg q(\bar{z}) \\ \forall \bar{z}\bar{u} T(\bar{z}\bar{u}) &\rightarrow R(\bar{z}\bar{u}) \\ \forall \bar{z}\bar{u} R(\bar{z}\bar{u}) &\rightarrow T(\bar{z}\bar{u}) \vee q(\bar{z}) \end{aligned}$$

Inner-most *equality-guarded* negations  $z = u \wedge \neg q(z, u)$  are handled in a similar fashion. Again,  $q(z, u)$  must be positive-existential. We choose a new unary relation symbol  $T$ , replace the subformula in question by  $z = u \wedge T(z)$ , and add  $\forall z T(z) \rightarrow \neg q[u/z]$  and  $\forall z T(z) \vee q[u/z]$  as conjuncts to the normal form, where  $q[u/z]$  is the formula constructed from  $q(z, u)$  by replacing all occurrences of  $u$  by  $z$ .

Proceeding in this manner from the inside-out we eliminate all guarded negations until the original input formula is reduced to a single positive-existential formula  $p(\bar{x})$  (in the extended signature). Finally we replace  $p(\bar{x})$  with  $S(\bar{x})$  where  $S$  is an appropriate new predicate symbol and add  $\forall \bar{x}. S(\bar{x}) \rightarrow p(\bar{x})$  as conjunct to the normal form, which is thus finalized. It is now easy to verify the correctness of this transformation.  $\square$

In view of Lemma 3.1, it remains to reduce the satisfiability problem of formulas in the form of (3) to the query answering problem against a GFO theory.

We may assume without loss of generality that the positive-existential formulas  $q_j$  of (3) are in prenex normal form, i.e.  $q_j(\bar{z}) = \exists \bar{u} \xi_j(\bar{z}, \bar{v})$  for some quantifier-free positive formula  $\xi_j(\bar{z}, \bar{v})$ . Also note that each conjunct  $\forall \bar{z}\bar{u} T_i(\bar{z}\bar{u}) \rightarrow \neg p_i(\bar{z})$  of (3) is the negation of a positive-existential

<sup>1</sup>In (3) the  $R_j$ 's and  $T_i$ 's are not necessarily distinct; moreover the size of the tuples  $\bar{z}$  and  $\bar{u}$  will in general vary from predicate to predicate and are denoted here uniformly by “ $\bar{z}$ ” and “ $\bar{u}$ ” only for sake of a simpler illustration.

sentence  $\exists \bar{z}\bar{u} T_i(\bar{z}\bar{u}) \wedge p_i(\bar{z})$ . Therefore, the entire  $\psi^-$  of (3) can be conceived as the negation of a single positive-existential sentence  $q$ . This leads us to the following equivalent formula.

$$\underbrace{S(\bar{x}) \wedge \bigwedge_j \left( \forall \bar{z}\bar{u} R_j(\bar{z}\bar{u}) \rightarrow \exists \bar{v} \xi_j(\bar{z}\bar{v}) \right)}_{\psi^+} \wedge \neg \underbrace{\bigvee_i \left( \exists \bar{z}\bar{u} T_i(\bar{z}\bar{u}) \wedge p_i(\bar{z}) \right)}_q \quad (4)$$

Observe next that without affecting satisfiability of (4) we may introduce new atoms guarding the existential quantifiers in  $\psi^+$  thus obtaining, from  $\psi^+$ , a GFO-formula

$$\psi^* = S(\bar{x}) \wedge \bigwedge_j \left( \forall \bar{z}\bar{u} R_j(\bar{z}\bar{u}) \rightarrow \exists \bar{v} Q_j(\bar{z}\bar{v}) \wedge \xi_j(\bar{z}\bar{v}) \right)$$

where the  $Q_j$ 's are distinct new relation symbols of appropriate arity. Then,  $\models \psi^* \rightarrow \psi^+$  and, conversely, every model of  $\psi^+$  has an expansion that is a model of  $\psi^*$ .

The entire transformation of an input GNFO-formula  $\varphi$  to the equi-satisfiable  $\psi^* \wedge \neg q$ , with  $\psi^*$  in GFO and  $q$  positive existential, can be performed in polynomial time and only results in a polynomial blowup in the signature of the latter formula. In a final transformation step, which may require at most exponential time, the positive-existential sentence  $q$  can be converted to an equivalent Boolean UCQ  $q^*$ . In general  $q^*$  may be comprised of exponentially many CQs each of size at most  $|q|$ . Summing up all the reduction steps we obtain:

**PROPOSITION 3.2.** *Given any formula  $\varphi(\bar{x}) \in \text{GNFO}[\tau]$  one can compute in exponential time a GFO-formula  $\psi^*(\bar{x})$  and UCQ  $q^*$ , both over a signature  $\tau \uplus \{\bar{T}\}$ , such that*

$$\models \varphi \longleftrightarrow \exists \bar{T} (\psi^* \wedge \neg q^*) \quad (5)$$

and such that  $|\psi^*|$  and  $\text{height}(q^*)$  are polynomial in  $|\varphi|$ .

We now summarize the main results of [Bárány et al. 2014]. Later we will build on key elements of the construction of [Bárány et al. 2014], stated below as Lemmas 4.6 and Theorem 4.13, from which the following Theorem 3.3 can be directly derived.

**THEOREM 3.3** ([BÁRÁNY ET AL. 2014]). *Given a GFO-formula  $\psi$  and a UCQ  $q$  of height  $h$  it is decidable in time  $|q| \cdot 2^{(h|\psi|)^{\mathcal{O}(h|\psi|)}}$  whether or not  $\psi \wedge \neg q$  is satisfiable; and if  $\psi \wedge \neg q$  has a model then it has a finite model of size  $2^{(h|\psi|)^{\mathcal{O}(h^2|\psi|)}}$*

By combining Theorem 3.3 with the estimates of Proposition 3.2 we derive the complexity of satisfiability for GNFO, as well as its finite model property.

**THEOREM 3.4.**

- (1) *The satisfiability problem for GNFO is 2EXPTIME-complete.*
- (2) *Every satisfiable GNFO-sentence  $\varphi$  has a finite model of size  $2^{2^{|\varphi|^{\mathcal{O}(1)}}}$ .*

#### 4. ADDING FIXPOINTS: THE SATISFIABILITY PROBLEM FOR GNFP

In this section, we introduce and study GNFP, which, in a nutshell, is the extension of GNFO with guarded fixpoints. We show that both satisfiability and finite satisfiability are decidable for GNFP.

**GNFP.** Guarded-negation fixpoint logic, GNFP, is a syntactic fragment of least fixpoint logic LFP, from which it inherits the semantics, cf. [Dawar and Gurevich 2002]. Recall that the syntax of LFP assumes an infinite supply of (second-order) fixpoint variables (denoted  $X, Y, Z, \dots$ ), of arbitrary arity. These fixpoint variables are distinct from the relation symbols that are in the relational signature (denoted  $P, Q, R, S, \dots$ ), and they serve for expressing fixpoints. Syntactically, they are

treated on a par with the ordinary relation symbols: they can be used in the same way in formulas. LFP then extends FO with the ability to construct formulas of the form

$$[\mu_{Z,\bar{z}} \phi(\bar{Y}, Z, \bar{z}, \bar{u})](\bar{x})$$

where  $Z$  is a fixpoint variable whose arity matches the length of sequences  $\bar{z}$  and  $\bar{x}$ , such that  $Z$  occurs only positive in  $\phi$  (i.e., all occurrences are under an even number of negation signs).

The guarded-negation fragment of LFP, called GNFP, is defined as follows:

*Definition 4.1.* Formulas of GNFP $[\tau]$ , we omit the signature  $\tau$  when it is clear from the context, pertain to the following syntax:

$$\phi ::= R(\bar{x}) \mid x = y \mid \phi_1 \wedge \phi_2 \mid \phi_1 \vee \phi_2 \mid \exists x \phi \mid \alpha(\bar{x}\bar{y}) \wedge \neg\phi(\bar{x}) \mid \\ \beta(\bar{u}\bar{w}) \wedge Z(\bar{u}) \mid \mu_{Z,\bar{z}}[\phi(\bar{Y}, Z, \bar{z})](\bar{x})$$

where  $R$  is any relational symbol in  $\tau$ ,  $\alpha(\bar{x}\bar{y})$  and  $\beta(\bar{u}\bar{w})$  are atomic  $\tau$ -formulas (possibly equality statements) and, in the last clause of the definition, the fixpoint variable  $Z$  occurs only positively in  $\phi(\bar{Y}, Z, \bar{z})$ , i.e. always under an even number of negations.

Note that

- no first-order parameters (i.e., free variables other than those  $\bar{z}$  bound by the fixpoint operator) are permitted in the matrix of a fixpoint operator,
- free fixpoint variables  $\bar{Y}$  other than  $Z$  are still allowed, enabling nesting and alternation of fixpoint definitions;
- fixpoint variables cannot be used as guards, and in fact, all atomic formulas involving fixpoint variables must be guarded by atomic  $\tau$ -formulas or equalities.

As we mentioned before, the semantics of GNFP is inherited from the logic LFP, of which it is a fragment. We briefly recall here the semantics of the fixpoint operator. Take a formula of the form

$$\mu_{Z,\bar{z}}[\phi(\bar{Y}, Z, \bar{z})](\bar{x})$$

and consider any structure  $(M, \bar{S})$ , where  $M$  is a structure over the relational signature and  $\bar{S}$  is a collection of relations over the domain of  $M$  (of suitable arity) that form the interpretation for the second-order variables  $\bar{Y}$ . Since  $Z$  occurs in  $\phi$  only positively,  $\phi(\bar{Y}, Z, \bar{z})$  induces a monotone operation  $\mathcal{O}_\phi$  on  $n$ -ary relations over the domain of  $M$ , where  $n$  is the arity of the fixpoint variable  $Z$ , and where  $\mathcal{O}_\phi(R) = \{\bar{a} \mid (M, \bar{S}, R) \models \phi(\bar{a})\}$ . By the Knaster-Tarski fixpoint theorem, this monotone operation has a unique least-fixpoint. By definition, an  $n$ -tuple  $\bar{b}$  of elements of  $M$  satisfies the formula  $[\mu_{Z,\bar{z}} \phi(\bar{Y}, Z, \bar{z})](\bar{x})$  in  $(M, \bar{S})$  if and only if  $\bar{b}$  belongs to this least fixpoint. The least fixpoint of the monotone operation  $\mathcal{O}_\phi$  is known to be the intersection of all its pre-fixpoints, i.e.,  $\bigcap \{R \mid R \supseteq \mathcal{O}_\phi(R)\}$ , and it can be equivalently characterized as  $\mathcal{O}_\phi^\kappa(\emptyset)$  with  $\kappa = |\text{dom}(M)|$ , where  $\mathcal{O}_\phi^0(\emptyset) = \emptyset$ ; for all successor ordinals  $\lambda + 1$ ,  $\mathcal{O}_\phi^{\lambda+1}(\emptyset) = \mathcal{O}_\phi(\mathcal{O}_\phi^\lambda(\emptyset))$ ; and for all limit ordinals  $\lambda \leq \kappa$ ,  $\mathcal{O}_\phi^\lambda(\emptyset) = \bigcup_{\lambda' < \lambda} \mathcal{O}_\phi^{\lambda'}(\emptyset)$ .

It is worth noting that, although the relation  $\mathcal{O}_\phi^\lambda(\emptyset)$  (for  $\lambda$  an ordinal) may contain unguarded tuples, the syntax of GNFP guarantees that the relation  $\mathcal{O}_\phi^{\lambda+1}(\emptyset)$  depends only on the  $\tau$ -guarded tuples in  $\mathcal{O}_\phi^\lambda(\emptyset)$ , and similarly for limit ordinals. In this sense, the fixpoint variables can be taken to range over guarded relations (i.e., relations consisting of guarded tuples only).

*Example 4.2.* The fixpoint formula

$$\mu_{Z,x,y}[E(x, y) \vee \exists z (Z(x, z) \wedge E(z, y))](u, v)$$

computing the transitive closure of  $E$  is not a formula of GNFP as the matrix formula does not guard the variables  $x, z$  occurring in  $Z(x, z)$ .

The fixpoint formula

$$\mu_{Z,z}[y = z \vee \exists y'(Z(y') \wedge E(y', y))](x)$$

computing the connected component of  $y$  is also not a formula of GNFP as the matrix formula has  $y$  as a parameter.

However the fixpoint formula

$$\mu_{Z,z}[B(z) \vee \exists y'(Z(y') \wedge E(y', z))](x)$$

computing the set of nodes reachable from a node in  $B$  is in GNFP as singletons are guarded by definition.

*Notes on syntax.* We could have defined GNFP with different alternative syntaxes of equivalent expressive power and varying degrees of succinctness. The variations concern how guardedness of fixpoint predicates is enforced. Let us briefly discuss the alternatives.

An ostensibly more restrictive syntax is obtained if we require that every fixpoint formula is to be guarded by a single atom of the base signature.

$$\mu_{Z,\bar{z}}[\alpha(\bar{z}) \wedge \phi(\bar{Y}, Z, \bar{z})](\bar{x}) \quad (6)$$

Notice how every formula of this form can be promptly rewritten in our syntax of choice as  $\mu_{Z,\bar{z}}[\phi^*(\bar{Y}, Z, \bar{z})](\bar{x})$  where  $\phi^*$  is obtained from  $\phi$  by replacing in it each atom  $Z(\bar{u})$  with the conjunction  $\alpha(\bar{u}) \wedge Z(\bar{u})$ . This transformation is obviously linear in the number of atoms.

In [Bárány et al. 2011] we presented GNFP using a similar pattern of fixpoint definitions

$$\mu_{Z,\bar{z}}[\text{guarded}_\tau(\bar{z}) \wedge \phi(\bar{Y}, Z, \bar{z})](\bar{x}) \quad (7)$$

where the clause  $\text{guarded}_\tau(\bar{z})$  is understood as a shorthand formula signifying guardedness in the signature  $\tau$  without expressly declaring any concrete guard. Notice that adding the special guardedness atom to a fixpoint definition in either of the two earlier forms does not affect the meaning of the formula but ensures compliance with this most liberal syntax. Conversely, to transcribe a formula adhering to syntax (7) one can replace each occurrence of an atom  $Z(\bar{z})$  involving a fixpoint predicate variable  $Z$  with the disjunction  $\bigvee_i \exists \bar{w}^i \alpha_i(\bar{w}^i \bar{z}) \wedge Z(\bar{z})$  where  $\bigvee_i \exists \bar{w}^i \alpha_i(\bar{w}^i \bar{z})$  spells out the definition of  $\text{guarded}_\tau(\bar{z})$ . This translation too is linear for any fixed signature, but is exponential in the maximum arity of relation symbols in the signature.

In order to show that syntax (6) does not restrict the expressive power of GNFP we shall temporarily avail ourselves of a further syntactic enhancement: that of *simultaneous fixpoint definitions*. Let again  $\bigvee_{1 \leq i \leq n} \exists \bar{w}^i \alpha_i(\bar{w}^i \bar{z})$  be the definition of guardedness of the tuple  $\bar{z}$  in signature  $\tau$ . To translate a fixpoint definition of the form (7) into (6) notation consider first the simultaneous fixpoint schema

$$\mu \left\{ \begin{array}{l} Z_1(\bar{w}^1 \bar{z}) \leftarrow \alpha_1(\bar{w}^1 \bar{z}) \wedge \phi'(\bar{Y}, \bar{Z}, \bar{z}) \\ \vdots \\ Z_n(\bar{w}^n \bar{z}) \leftarrow \alpha_n(\bar{w}^n \bar{z}) \wedge \phi'(\bar{Y}, \bar{Z}, \bar{z}) \end{array} \right\}$$

where now  $Z$  has been replaced with a tuple  $\bar{Z} = Z_1, \dots, Z_n$  of fixpoint variables, one for each disjunct in the definition of guardedness, with each  $Z_i$  of arity  $|\bar{w}^i| + |\bar{z}|$ , and where  $\phi'$  is obtained by replacing in  $\phi$  every occurrence of an atom  $Z(\bar{u})$  with the disjunction  $\bigvee_i \exists \bar{w}^i Z_i(\bar{w}^i \bar{u})$ . Notice how the definition of each fixpoint predicate variable  $Z_i$  is guarded according to the pattern (6). This simultaneous fixpoint can be transformed using the Bekič principle, cf. e.g. [Arnold and Niwinski 2001], with a formula for each of the alternative  $Z_i$

$$\mu_{Z_i, \bar{w}^i, \bar{z}} [\alpha_i(\bar{w}^i \bar{z}) \wedge \phi_i^*(\bar{Y}, \bar{Z}, \bar{z})]$$

pertaining to (6). Finally, the original fixpoint formula as in (7) is rewritten to

$$\bigvee_i \exists \bar{w}^i \mu_{Z_i, \bar{w}^i, \bar{z}} [\alpha_i(\bar{w}^i \bar{z}) \wedge \phi_i^*(\bar{Y}, \bar{Z}, \bar{z})](\bar{u}^i \bar{x})$$

and this rewriting is to be applied recursively to formulas with nested fixpoint definitions. Notice how this translation of formulas from dialect (7) to dialect (6) of GNFP will thus produce exponen-

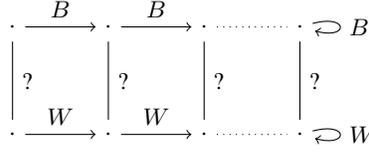


Fig. 1. Illustration of the example fixpoint formula

tially long formulas in terms of the number of nested fixpoints in the formula started with, even if we fix the signature.

To illustrate this translation consider the example, over graphs with black and white edges, provided by the formula  $\rho(p, q)$  defined as

$$\mu_{Z,x,y} \left[ \text{guarded}_{\{B,W\}}(x, y) \wedge (\exists uv (B(x, u) \wedge W(y, v) \wedge Z(u, v)) \vee (B(x, x) \wedge W(y, y))) \right] (p, q)$$

expressing the existence of two parallel paths, one black the other white, forming a reel of conjoined cells ending in adjacent vertices with a black and a white self-loop, respectively (cf. Figure 1). First observe that  $\text{guarded}_{\{B,W\}}(x, y)$  is equivalent to the disjunction  $B(x, y) \vee W(x, y) \vee B(y, x) \vee W(y, x) \vee x = y$ . Correspondingly, we construct a simultaneous fixpoint schema consisting of five equations:

$$\mu \left\{ \begin{array}{l} Z_1(x, y) \leftarrow B(x, y) \wedge \exists uv (B(x, u) \wedge W(y, v) \wedge (\bigvee_i Z_i(u, v))) \vee (B(x, x) \wedge W(y, y)) \\ Z_2(x, y) \leftarrow W(x, y) \wedge \exists uv (B(x, u) \wedge W(y, v) \wedge (\bigvee_i Z_i(u, v))) \vee (B(x, x) \wedge W(y, y)) \\ \vdots \end{array} \right\}$$

To simplify the notation and keep the example comprehensible, we will (against better knowledge) pretend that the fixpoint schema we constructed consists only of the two formulas for  $Z_1$  and  $Z_2$  spelled out above. Then, eliminating the simultaneous fixpoint definition results in two nested fixpoint formulas, first

$$\zeta_1(p, q) = \mu_{Z_1,x,y} [B(x, y) \wedge \exists uv (B(x, u) \wedge W(y, v) \wedge (Z_1(u, v) \vee \xi_2(Z_1, u, v))) \vee (B(x, x) \wedge W(y, y))] (p, q)$$

where

$$\xi_2(Z_1, u, v) = \mu_{Z_2,\hat{x},\hat{y}} [W(\hat{x}, \hat{y}) \wedge \exists \hat{u}\hat{v} (B(\hat{x}, \hat{u}) \wedge W(\hat{y}, \hat{v}) \wedge (Z_1(\hat{u}, \hat{v}) \vee Z_2(\hat{u}, \hat{v})) \vee (B(\hat{x}, \hat{x}) \wedge W(\hat{y}, \hat{y}))) (u, v)$$

and, symmetrically,

$$\zeta_2(p, q) = \mu_{Z_2,x,y} [W(x, y) \wedge \exists uv (B(x, u) \wedge W(y, v) \wedge (Z_1(u, v) \vee \xi_1(Z_2, u, v))) \vee (B(x, x) \wedge W(y, y))] (p, q)$$

where

$$\xi_1(Z_2, u, v) = \mu_{Z_1,\hat{x},\hat{y}} [B(\hat{x}, \hat{y}) \wedge \exists \hat{u}\hat{v} (B(\hat{x}, \hat{u}) \wedge W(\hat{y}, \hat{v}) \wedge (Z_1(\hat{u}, \hat{v}) \vee Z_2(\hat{u}, \hat{v})) \vee (B(\hat{x}, \hat{x}) \wedge W(\hat{y}, \hat{y}))) (u, v)$$

corresponding to the cases of reels starting in a black and in a white cross edge, respectively.

Finally, the original black and white reel formula  $\rho(p, q)$  is transcribed into the equivalent formula  $\bigvee_i \zeta_i(p, q)$ , which adheres to the most restrictive of the three alternative syntaxes for GNFP discussed above, i.e., the syntax given in (6).

This example also illustrates the fact that allowing simultaneous fixpoint schemas in GNFP formulas does not increase the expressive power of the logic (although it can facilitate more succinct definitions).

We have opted for the syntax of definition 4.1 because it allows for more intuitive formulas than (6) while also avoiding a penalty of increased complexity of model checking that the most liberal syntax (7) entails, as discussed in Section 5.

The definition of GN-normal form that we gave for GNFO formulas applies to GNFP as well. Formulas of GNFP in GN-normal form can be naturally thought of as being built up from atomic formulas using (i) guarded negation, (ii) unions of conjunctive queries, and (iii) fixpoint operators. As in the case of GNFO, the *width* of a GNFP-formula is the number of variables it contains after being put in GN-normal form and we let  $\text{GNFP}^k$  denote the set of GNFP-formulas of width  $k$ .

**GNFP extends GFP and UNFP.** Syntactically, GNFP generalizes the logic UNFP studied in [ten Cate and Segoufin 2013], which only allows the negation of formulas having at most one free variable, and only unary fixpoints. GNFP also generalizes the *guarded fragment of fixpoint logic* (GFP) [Grädel and Walukiewicz 1999], in the sense that every sentence of GFP is equivalent to a sentence of GNFP.

Recall that GFP is the fragment of LFP obtained by extending GFO with least fixpoints: given a formula  $\phi(\bar{Y}, Z, \bar{z})$  that is positive in  $Z$ , has no free first-order variables other than  $\bar{z}$  and  $Z$  has arity the number of variables in  $\bar{z}$ , the formula  $\mu_{Z, \bar{z}}[\phi(\bar{Y}, Z, \bar{z})]$  is also a formula of GFP. Although the occurrences of fixpoint variables are not required to be guarded, in the context of a GFP *sentence*, every occurrence of an atom using a fixpoint relation is implicitly guarded, namely by the atom guarding the closest quantifier whose scope includes the occurrence in question). This implies:

**PROPOSITION 4.3.** *Every sentence of GFP is equivalent to a sentence of GNFP, via a polynomial time transformation.*

**GNFP is decidable.** The aim of this section is to establish the following main result.

**THEOREM 4.4.** *It is decidable whether a sentence of GNFP has a model and whether it has a finite model. Both of these problems are 2EXPTIME-complete.*

The proof of Theorem 4.4 is a reduction to the (finite) satisfiability of GFP: given a formula of GNFP we construct a formula of GFP whose (finite) satisfiability is equivalent to the one of the initial formula and we then apply known results on (finite) satisfiability for GFP, namely [Grädel and Walukiewicz 1999] for the infinite case and [Bárány and Bojańczyk 2012] for the finite case. Before we describe the reduction, we start with some useful notation and some preliminary results taken from [Bárány et al. 2014].

**Acyclic structures, acyclic queries, and treeifications.** A structure  $M$  is said to be *acyclic* if it admits a *guarded tree decomposition*, that is, a tree decomposition each bag of which belongs to  $\text{guarded}(M)$  [Yannakakis 1981; Flum et al. 2002]. We omit here the definition of tree decomposition, which can be found e.g. in [Flum et al. 2002], as it turns out not to be important in what follows. The above definition of acyclicity extends also to *conjunctive queries*. Formally, we associate to each query  $q(\bar{x})$  a structure  $[q]$ , called the *canonical structure* of  $q$ , whose nodes are the variables occurring in  $q$ , and whose facts are the atoms of  $q$ . A conjunctive query is *acyclic* if its canonical structure has a guarded tree decomposition. Acyclic conjunctive queries have been studied extensively in database theory, and have been shown to have many desirable properties [Yannakakis 1981]. Every acyclic conjunctive query can be equivalently rewritten (in polynomial time) as a formula of GFO built with only conjunction and existential quantification, and, conversely, every such GFO formula can be rewritten (in polynomial time) as an acyclic conjunctive query [Flum et al. 2002]. For instance the query  $\exists yzw T(x, y, z) \wedge T(x, w, z) \wedge E(x, y)$  is acyclic because it is equivalent to the guarded formula  $\exists yz T(x, y, z) \wedge E(x, y) \wedge (\exists w T(x, w, z))$ .

**Definition 4.5 (Treeification).** Given a signature  $\tau$ , the  $\tau$ -*treeification*  $\Lambda_q^\tau(\bar{x})$  of a positive existential query  $q(\bar{x})$  over  $\tau$  is the UCQ consisting of the disjunction of all those *acyclic* CQs over  $\tau$  (modulo renaming of bound variables) that imply  $q$  and that are minimal (in the sense that removing any atomic formula would render it non-acyclic or not implying  $q$ ).

Lemma 4.6 below will justify this definition by showing that there are only finitely many minimal acyclic conjunctive queries (up to logical equivalence) that imply a given query  $q$ .

First we give an example. Consider the conjunctive query  $q(x)$  defined as

$$\exists yzw (E(x, y) \wedge E(y, z) \wedge E(z, w) \wedge E(w, x)).$$

Then its  $\{E\}$ -treeification  $\Lambda_q^{\{E\}}$  is the formula

$$E(x, x) \vee \exists y (E(x, y) \wedge E(y, x)).$$

Indeed, the only minimal acyclic queries implying  $q(x)$  are obtained by identifying some of its variables resulting in either a reflexive edge on  $x$  or a pair of inverse edges. If the signature is  $\{E, T\}$ , where  $T$  is a ternary predicate, the treeification of  $q(x)$  has a number of additional disjuncts corresponding to various triangulations of  $q(x)$ , such as

$$\exists yzw (T(x, y, z) \wedge T(x, w, z) \wedge E(x, y) \wedge E(y, z) \wedge E(z, w) \wedge E(w, x))$$

(which is acyclic because it is equivalent to  $\exists yz (T(x, y, z) \wedge E(x, y) \wedge E(y, z) \wedge \exists w ((T(x, w, z) \wedge E(z, w) \wedge E(w, x)))$ ). It can be shown that each disjunct in the treeification of any CQ in whatever signature contains at most three times as many atoms as the CQ itself [Bárány et al. 2014] leading to the following observations.

**LEMMA 4.6.** *Consider a signature  $\tau$  having  $r$  many predicate symbols of maximal arity  $w$ . Let  $q(\bar{x})$  be a UCQ of height  $h$  over  $\tau$ . Then  $\Lambda_q^\tau(\bar{x})$  has width  $w$ , size  $r^{\mathcal{O}(h)}(hw)^{\mathcal{O}(hw)}$ , height  $\mathcal{O}(hw)$ , and can be constructed in time  $|q|r^{\mathcal{O}(h)}(hw)^{\mathcal{O}(hw)}$ .*

These figures constitute a slight refinement of those offered in [Bárány et al. 2014, Lemma 10], where it was shown that every disjunct  $T$  in the treeification of  $Q$  has at most  $c = 3$  times as many atoms as  $Q$ , whence the prenex normal form of  $T$  involves at most  $c|Q|w$  many variables and has size  $\mathcal{O}(|Q|w)$ . In fact, one can check that  $c = 2$  suffices and that the number of CQs of these dimensions is at most  $(r(c|Q|w)^w)^{c|Q|}$ . Note that when writing  $T$  as a guarded formula only  $w$  many variables are needed and the resulting formula is still of size  $\mathcal{O}(|Q|w)$ . Because each acyclic CQ as above may occur (modulo renaming of bound variables) at most once in  $\Lambda_Q^\tau$ , we find that  $|\Lambda_Q^\tau| = (r(c|Q|w)^w)^{c|Q|} \mathcal{O}(|Q|w) = r^{\mathcal{O}(|Q|)}(|Q|w)^{\mathcal{O}(|Q|w)}$ , the width of  $\Lambda_Q^\tau$  is  $w$ , and its height is  $\mathcal{O}(|Q|w)$ .

*Remark 4.7.* Over acyclic structures,  $q$  and  $\Lambda_q^\tau$  are equivalent. Indeed consider a conjunctive query  $q$  and an acyclic structure  $M$  such that  $M \models q(\bar{b})$ . Then there is an homomorphism  $f$  from  $q$  to  $M$ . The image  $f(q)$  can be viewed as an acyclic conjunctive query that clearly implies  $q$ .

In general  $q$  and  $\Lambda_q^\tau$  are not equivalent but we will use structures that are locally sufficiently acyclic such that equivalence is achieved for small queries  $q$ . This suggests the following definition:

**Definition 4.8 (Allowing for treeifications).** A  $\tau$ -structure  $M$  allows for treeifications of width  $n$  if for every conjunctive query  $q$  of width  $n$  and tuple  $\bar{b}$  guarded in  $M$ , we have

$$M \models q(\bar{b}) \leftrightarrow \Lambda_q^\tau(\bar{b}).$$

We now discuss ways of obtaining structures that allow for treeifications using *guarded bisimulations*. Guarded bisimulations [Andréka et al. 1998] form a fundamental tool in the study of guarded logics. In particular, the existence of a guarded bisimulation implies GFP-indistinguishability [Grädel 1999a]. We briefly review guarded bisimulations and some of their applications here. Later, in Section 6, we will introduce *guarded-negation bisimulations* in order to capture, in the same way, the expressive power of GNFP.

Recall the notion of a guarded tuple and the notation  $\textit{guarded}(M)$  from Section 2.

*Definition 4.9 (Guarded bisimulation).* Let  $M, N$  be two structures. A guarded bisimulation between  $M$  and  $N$  is a binary relation  $Z \subseteq \text{guarded}(M) \times \text{guarded}(N)$  such that, for every pair  $(\bar{a}, \bar{b}) \in Z$ , where  $\bar{a} = a_1, \dots, a_m$  and  $\bar{b} = b_1, \dots, b_n$ , the following conditions hold:

- $(M, \bar{a})$  and  $(N, \bar{b})$  are locally isomorphic (that is,  $m = n$  and the relation  $\{(a_i, b_i) \mid 1 \leq i \leq n\}$  is the graph of a partial isomorphism between  $M$  and  $N$ ).
- **[Forward clause]** For every tuple  $\bar{a}'$  in  $\text{guarded}(M)$  there is a tuple  $\bar{b}'$  in  $\text{guarded}(N)$  such that  $(\bar{a}', \bar{b}') \in Z$  and, whenever  $a'_i = a_i$  for some  $i \leq n$  then also  $b'_i = b_i$ .
- **[Backward clause]** For every tuple  $\bar{b}'$  in  $\text{guarded}(N)$  there is a tuple  $\bar{a}'$  in  $\text{guarded}(M)$  such that  $(\bar{a}', \bar{b}') \in Z$  and, whenever  $b'_i = b_i$  for some  $i \leq n$  then also  $a'_i = a_i$ .

**THEOREM 4.10** ([ANDRÉKA ET AL. 1998; GRÄDEL 1999A]).

*If  $Z$  is a guarded bisimulation between structures  $M$  and  $N$ , and  $(\bar{a}, \bar{b}) \in Z$ , then, for all GFP-formulas  $\phi(\bar{x})$ ,  $M \models \phi[\bar{a}]$  iff  $N \models \phi[\bar{b}]$ .*

One important consequence of Theorem 4.10 is that GFP has the *tree-like model property*: every satisfiable GFP-formula has an acyclic model. This follows from Theorem 4.10, because every structure is guarded bisimilar to an acyclic structure [Andréka et al. 1998; Grädel 2001].

Even though every structure is guarded bisimilar to an acyclic structure, the latter is in general infinite even if the original structure was finite. For example, let  $M$  be the structure that consists of a directed  $R$ -cycle of length 3 (where  $R$  is a binary relation symbol). It is easy to see that every acyclic structure  $M'$  that is guarded bisimilar to  $M$  must contain an infinite  $R$ -path, and no reflexive or symmetric  $R$ -edges. It follows that, if  $M'$  is finite, then it must contain some minimal directed  $R$ -cycle of length at least 3. This shows that  $M'$  cannot be finite and acyclic at the same time.

To address this problem, in [Bárány et al. 2014], a construction was presented, parametrized by a natural number  $n$ , that takes any finite structure  $M$  and produces a “weakly  $n$ -acyclic” finite companion structure  $M^{(n)}$  that is guarded bisimilar to  $M$  and that allows for treeifications of conjunctive queries of width at most  $n$ . To state the result formally, we need the concept of *guarded bisimilar covers* due to [Otto 2004], cf. [Bárány et al. 2014, Definition 1].

*Definition 4.11 (Guarded bisimilar cover).* A guarded bisimilar cover  $\pi: N \xrightarrow{\sim} M$  is a surjective homomorphism  $\pi: N \rightarrow M$  such that the induced map  $\{(\bar{b}, \pi(\bar{b})) \mid \bar{b} \text{ guarded in } N\}$  is a guarded bisimulation. A cover  $\pi: N \xrightarrow{\sim} M$  is *weakly  $k$ -acyclic* if for every homomorphism  $h: Q \rightarrow N$  with  $|Q| \leq k$  the composition  $\pi \circ h$  factors as  $g \circ f$  for some homomorphisms  $f: Q \rightarrow T$  and  $g: T \rightarrow M$  where  $T$  is acyclic.

Note that, in the above, if  $Q$  is the *canonical structure*  $[q]$  of a CQ  $q$  and  $t$  is the acyclic CQ such that  $T = [t]$  then we have  $t \models q$ . Therefore, in the above  $T$  can wlog. be chosen with  $t$  corresponding to a disjunct of the treeification of  $q$ . The following is thus a straightforward corollary of (and motivation for) the definitions involved.

**FACT 4.12.** *If  $\pi: N \xrightarrow{\sim} M$  is a weakly  $k$ -acyclic guarded bisimilar cover of  $M$  then (i)  $M$  and  $N$  have identical GFP theories and (ii)  $N$  allows for treeifications of width  $k$ .*

**PROOF.** The first claim is a corollary of guarded bisimulation invariance of GFP. For the second claim, consider  $N \models q(\bar{b})$  for some guarded tuple  $\bar{b}$  and a CQ  $q(\bar{x})$  of width at most  $k$ . Let  $h: [q] \rightarrow N$  be the homomorphism witnessing this. Then, by definition of weak  $k$ -acyclicity we have  $\pi \circ h = g \circ f$  for homomorphisms  $f: [q] \rightarrow [t]$  and  $g: [t] \rightarrow M$  where  $t$  is some acyclic CQ. In particular, we have that  $t(\bar{x}) \models q(\bar{x})$  and that  $M \models t(\pi(\bar{b}))$ . Note that as such  $t$  can be chosen to be minimal (in terms of number of atoms) and thus a disjunct of the treeification  $\Lambda_q(\bar{x})$  of  $q(\bar{x})$ . Also, by guarded bisimulation invariance of acyclic conjunctive queries we get that  $N \models t(\bar{b})$ , whence  $N \models \Lambda_q(\bar{b})$ .  $\square$

The following technical result will play a key role in our argument.

**THEOREM 4.13** ([BÁRÁNY ET AL. 2014, THEOREM 4]). *For every finite relational structure  $M$  and every  $n \in \mathbb{N}$  one can effectively construct a weakly  $n$ -acyclic guarded bisimilar cover  $\pi: M^{(n)} \xrightarrow{\sim} M$  of size  $|M^{(n)}| = |M|^{w^{O(n^2)}}$ , where  $w$  is the maximal arity of the relations of  $M$ . Furthermore,  $M^{(n)}$  is  $n$ -conformal, meaning that every clique-guarded tuple of  $M^{(n)}$  of size at most  $n$  is guarded.  $M^{(n)}$  is called the  $n$ -th Rosati cover of  $M$ .*

The last assertion of Theorem 4.13 requires some explanation. We say that a tuple  $\bar{b}$  of elements of a structure is *clique-guarded* if for every pair  $b_i, b_j \in \bar{b}$ ,  $b_i$  and  $b_j$  co-occur in an atomic fact. Note that every guarded tuple is clique-guarded. The  $n$ -conformality expresses a restricted form of the converse direction, which will be put to use later on, in Section 7.1.

Fact 4.12 asserts that weakly  $k$ -acyclic covers allow for treeifications of width  $k$ . The next lemma identifies conditions under which this key property extends to suitable expansions of the base structure and of the cover. Below we use this observation in our inductive argument for Lemma 4.16 concerning GNFP-formulas with free fixpoint variables.

Say that  $Z \subseteq M^r$  is a *guarded relation* over  $M$  if every tuple  $\bar{a} \in Z$  is guarded in  $M$ . Given a cover  $\pi: N \xrightarrow{\sim} M$ , say that a guarded relation  $W \subseteq N^r$  is  $\pi$ -*saturated* if  $W = \pi^{-1}(\pi(W)) \cap \text{guarded}(N)$ , viz. if  $W = \pi^{-1}(Z) \cap \text{guarded}(N)$  for some guarded relation  $Z$  over  $M$ .

**LEMMA 4.14.** *Consider a weakly  $(wn^w)$ -acyclic guarded bisimulation cover  $\pi: N \xrightarrow{\sim} M$  of some relational  $\tau$ -structure  $M$ , where  $w$  is the maximal arity of the relation symbols in the signature  $\tau$ .<sup>2</sup> Let  $Z_1, \dots, Z_t$  be guarded relations over  $M$  and for each  $1 \leq i \leq t$  let  $W_i = \pi^{-1}(Z_i) \cap \text{guarded}(N)$ . Then  $(N, W_1, \dots, W_t)$  allows for treeifications of width  $n$ .*

**PROOF.** We write  $\widehat{N}$  for  $(N, W_1, \dots, W_t)$  and  $\widehat{M}$  for  $(M, Z_1, \dots, Z_t)$ . Let  $\tau$  denote the signature of  $N$  and  $M$  and  $\sigma$  the signature of  $\widehat{N}$  and  $\widehat{M}$ . We first observe that  $\pi$  remains a guarded bisimilar cover from  $\widehat{N}$  to  $\widehat{M}$ . This is an immediate consequence of the fact that the  $Z_i$  are guarded relations and the  $W_i$  are  $\pi$ -saturated.

Consider now a conjunctive query  $q(\bar{x})$  of width  $n$  in the signature  $\sigma$  and a guarded tuple  $\bar{b}$  of elements of  $\widehat{N}$  such that  $\widehat{N} \models q(\bar{b})$ . We need to show that  $\widehat{N} \models \Lambda_q^\sigma(\bar{b})$ .

Let  $h: [q], \bar{x} \rightarrow \widehat{N}, \bar{b}$  be a homomorphism witnessing  $\widehat{N} \models q(\bar{b})$ . Consider an atom  $\alpha$  of  $q$  whose symbol is in  $\sigma \setminus \tau$ . Its image by  $h$  is a tuple  $\bar{c}$  from  $W_l$  for  $l$  as specified by  $\alpha$ . Since by assumption the relations  $W_l$  are guarded in  $N$ ,  $\bar{c}$  is guarded by a tuple  $\bar{d}$  occurring in some relation  $R$  of  $N$ .

Let  $R(\bar{z})$  be a new atom such that for all  $i$ ,  $z_i$  is the smallest variable  $y_j$  of  $\alpha$  such that  $h(y_j) = d_i$  or let  $z_i$  be a fresh new variable if there is no such  $y_j$ . We denote this atom by  $\alpha[h, \tau]$ . Let  $Q$  be the query in the signature  $\tau$  constructed from  $q$  by omitting all its atoms  $\alpha$  whose symbol is in  $\sigma \setminus \tau$ , replacing each by  $\alpha[h, \tau]$ , and by quantifying existentially all the fresh new variables. By construction,  $h$  can be extended to a homomorphism  $H: ([Q], \bar{x}) \rightarrow (N, \bar{b})$ .

Wlog. we may assume that the atoms  $\alpha$  of  $q$  being replaced are pairwise incomparable, so that no one is contained inside another (otherwise we may freely omit the replacement of the smaller one from  $Q$ ). Also note that the assumptions of the lemma imply that each  $W_i$  is of arity at most  $w$ . The number of (maximal) atoms  $\alpha$  of  $q$  thus being replaced is no more than  $n^w$ , so that  $Q$  has at most that many replacement atoms  $\alpha[h, \tau]$ , each contributing at most  $w - 1$  new variables. The width of  $Q$  is therefore not greater than the original  $n$  plus  $(w - 1)n^w$ , not more than  $wn^w$ .

Let  $q'$  be the conjunctive query in the signature  $\sigma$  obtained by adding to  $q$  the conjunct  $\alpha[h, \tau]$  for all (maximal)  $\sigma \setminus \tau$ -atoms  $\alpha$  and quantifying existentially all the fresh new variables. Note that  $q'$  implies  $Q$  and also implies  $q$ , that  $[q']$  has the same domain as  $[Q]$  and that  $H$  also witnesses  $\widehat{N} \models q'(\bar{b})$ . Our aim is to show  $\widehat{N} \models \Lambda_{q'}^\sigma(\bar{b})$  from which  $\widehat{N} \models \Lambda_q^\sigma(\bar{b})$  will follow trivially.

<sup>2</sup>A slightly more meticulous argument operating at the level of the underlying hypergraphs, as in [Bárány et al. 2014], would allow one to accurately establish the tight weak acyclicity bound of  $n$  in place of the  $(wn^w)$  stated here.

Let  $\bar{a} = \pi(\bar{b})$ . By construction we have  $H' = \pi \circ H$  maps  $[Q], \bar{x}$  into  $M, \bar{a}$ . By virtue of Fact 4.12 it holds that  $M \models \Lambda_Q^\tau(\bar{a})$ , witnessed by a homomorphism  $G': [T], \bar{x} \rightarrow M, \bar{a}$ , with  $T$  a disjunct of  $\Lambda_Q^\tau$  such that  $H' = G' \circ F$  for some  $F: [Q(\bar{x})] \rightarrow [T(\bar{x})]$ .

Let  $t'$  be constructed from  $T$  by adding to  $T$  the conjunct  $F(\alpha)$  for every atom  $\alpha \in \sigma \setminus \tau$  in  $q$  (hence also in  $q'$ ). By construction  $t'$  remains acyclic and  $F: [q'(\bar{x})] \rightarrow [t'(\bar{x})]$ , which means that  $t'$  implies  $q'$ . Recall that  $H$  also witnesses the fact that  $\widehat{N} \models q'(\bar{b})$  and therefore  $H'$  witnesses the fact that  $\widehat{M} \models q'(\bar{a})$ . As  $H' = G' \circ F$  and  $F: [q'(\bar{x})] \rightarrow [t'(\bar{x})]$ , it must be the case that  $G'$  witnesses the fact that  $\widehat{M} \models t'(\bar{a})$ . Altogether we have shown that  $t'(\bar{x})$  is an acyclic CQ that implies  $q'(\bar{x})$  and that is satisfied in  $\widehat{M}$  by  $\bar{a}$ . Therefore  $G' \circ F$  witnesses  $\widehat{M} \models \Lambda_{q'}^\sigma(\bar{a})$ . As  $\Lambda_{q'}^\sigma$  is acyclic it is invariant under guarded bisimulation and, therefore, from  $\widehat{M} \models \Lambda_{q'}^\sigma(\bar{a})$  we get  $\widehat{N} \models \Lambda_{q'}^\sigma(\bar{b})$  as desired.  $\square$

**Reduction to (finite) satisfiability for GFP.** Let  $\varphi$  be any given GNFP sentence. As a first step, we compute its GN-normal form  $\tilde{\varphi}$ . Note that  $\tilde{\varphi}$  has the following dimensions:  $|\tilde{\varphi}| = 2^{\mathcal{O}(|\varphi|)}$ ,  $\text{width}(\tilde{\varphi}) = \mathcal{O}(|\varphi|)$ , and  $\tilde{\varphi}$  is built up using only UCQs of height at most  $|\varphi|$  (as well as guarded negations and fixpoint operators) as in (2).

Next, essentially, our reduction transforms all UCQs occurring in  $\tilde{\varphi}$  to their treeifications. For every  $k \geq 1$ , and for every relational signature  $\tau$  consisting of at most  $k$ -ary relations, we define a translation  $\eta$  from  $\text{GNFP}^k[\tau]$  formulas in GN-normal form to  $\text{GFP}^k[\tau \uplus \{C_k\}]$  formulas, where  $C_k$  is a new symbol of arity  $k$ , by structural recursion, using the following rules.

$$\eta(R(\bar{x})) = R(\bar{x}) \tag{a}$$

$$\eta(\alpha(\bar{x}\bar{y}) \wedge Z(\bar{x})) = \alpha(\bar{x}\bar{y}) \wedge Z(\bar{x}) \tag{b}$$

$$\eta(\alpha(\bar{x}\bar{y}) \wedge \neg\psi(\bar{x})) = \alpha(\bar{x}\bar{y}) \wedge \neg\eta(\psi(\bar{x})) \tag{c}$$

$$\eta(\mu_{Z,\bar{z}}[\psi(\bar{Y}, Z, \bar{z})]) = \mu_{Z,\bar{z}}[\eta(\psi(\bar{Y}, Z, \bar{z}))] \tag{d}$$

$$\eta(q[\phi_1/U_1, \dots, \phi_s/U_s]) = \Lambda_q^{\tau \uplus \{U_1, \dots, U_s, C_k\}}[\eta(\phi_1)/U_1, \dots, \eta(\phi_s)/U_s] \tag{e}$$

where in (e)  $q$  is a UCQ of signature  $\{U_1, \dots, U_s\}$  disjoint from  $\tau \uplus \{\bar{Y}, C_k\}$  and  $\phi_1, \dots, \phi_s \in \text{GNFP}^k[\tau \uplus \{\bar{Y}\}]$ , where  $\bar{Y}$  enumerates the free fixpoint variables occurring in any of the  $\phi_i$ 's, each  $\phi_i$  being a guarded formula.

By (2) all formulas in GN-normal form can be decomposed as in (a)–(e) and we have the following bounds on the translation  $\eta$ .

**LEMMA 4.15.** *For every  $\text{GNFP}^k$ -formula  $\varphi$  with GN-normal form  $\tilde{\varphi}$  we have  $|\eta(\tilde{\varphi})| = 2^{(k|\varphi|)^{\mathcal{O}(1)}}$  and  $\eta(\tilde{\varphi})$  can be computed within this time bound and its width remains  $k$ .*

**PROOF.** To establish the bound  $|\eta(\tilde{\varphi})| = 2^{(k|\varphi|)^{\mathcal{O}(1)}}$  we proceed via structural induction on  $\varphi$  following the definition of the translation  $\eta$  according to the cases (a)–(e) and using as invariant the claim  $|\eta(\tilde{\psi})| \leq 2^{c|\tau|k^2|\psi|^3}$ , where  $c$  is an appropriate constant to be fixed later. The claim of the lemma follows assuming wlog. that  $|\tau| \leq |\varphi|$ .

Irrespective of  $c$  this bound trivially holds for all atomic formulas whether based on a  $\tau$ -predicate (a) or a fixpoint variable (b). It is also plain to see that assuming  $|\eta(\tilde{\psi})| = 2^{c|\tau|k^2|\psi|^3}$  the same bound holds for (c) all guarded-negation formulas of the form  $\alpha(\bar{x}\bar{y}) \wedge \neg\psi(\bar{x})$ , as well as for (d) least fixpoint formulas  $\mu_{Z,\bar{z}}[\psi(\bar{Y}, Z, \bar{z})]$ . In each of these cases  $\eta(\tilde{\psi})$  is computable in  $2^{(k|\psi|)^{\mathcal{O}(1)}}$ -time, assuming the same for the relevant subformulas of  $\psi$ .

The remaining case is when  $\tilde{\varphi}$  is  $q[\tilde{\phi}_1/U_1, \dots, \tilde{\phi}_s/U_s]$  for  $q$  a UCQ and  $\phi_1, \dots, \phi_s$  subformulas of  $\varphi$ . We have already noted that the height  $h$  of  $q$  is no more than  $|\varphi|$ , and the same holds for  $s$  too. Further, by design we know that the maximum arity of the predicates among  $\tau \uplus \{U_1, \dots, U_s, C_k\}$  is  $k$ . Therefore, using Lemma 4.6, we have  $|\Lambda_q^{\tau \uplus \{U_1, \dots, U_s, C_k\}}| = (|\tau| + s + 1)^{\mathcal{O}(h)} (kh)^{\mathcal{O}(kh)} \leq$

$2^{c|\tau|(k|\varphi|^2)}$  for some constant  $c$ . By the induction hypothesis for each  $1 \leq i \leq s$  we have  $|\eta(\tilde{\phi}_i)| \leq 2^{ck^2|\phi_i|^3}$ . Let  $l = \max_i |\phi_i| < |\psi|$ . Then the size of  $\eta(\tilde{\varphi})$ , obtained by substituting  $\tilde{\phi}_i$  for  $U_i$  for every  $1 \leq i \leq s$  in  $\Lambda_q^{\tau \uplus \{U_1, \dots, U_s, C_k\}}$ , is bounded by  $2^{c|\tau|(k|\varphi|^2)} \cdot 2^{c|\tau|k^2l^3} \leq 2^{c|\tau|k^2|\varphi|^2(l+1)} \leq 2^{c|\tau|k^2|\varphi|^3}$ . That  $\eta(\tilde{\varphi})$  can be computed in the stated time bound also for  $\varphi$  of type (e) follows similarly using Lemma 4.6.  $\square$

The following key lemma attests to the correctness of our reduction. It is proved by structural induction on formulas, while relying on Theorem 4.13 and Lemma 4.14 to deal with the cases (d) and (e) of the translation, respectively.

LEMMA 4.16. *Let  $\pi : N \xrightarrow{\sim} M$  be a weakly ( $wk^w$ )-acyclic guarded bisimulation cover of a  $\tau \uplus \{C_k\}$ -structure  $M$ , where  $w$  is the maximal arity of the symbols of  $\tau \uplus \{C_k\}$  and let  $\phi(\bar{Y}, \bar{x}) \in \text{GNFP}^k[\tau]$  be a formula in GN-normal form with free fixpoint variables  $\bar{Y}$ . Then for every interpretation of  $\bar{Y}$  by  $\pi$ -saturated<sup>3</sup> guarded relations  $\bar{W}$  on  $N$  and for every guarded tuple  $\bar{b}$  in  $N$  we have:*

$$(N, \bar{W}) \models \eta(\phi)(\bar{b}) \leftrightarrow \phi(\bar{b}).$$

PROOF. We proceed by induction on the structure of  $\phi$ , wlog. in GN-normal form. The base case is trivial since  $\phi = \eta(\phi)$  for all atomic formulas. Moreover, the claim trivially distributes over positive Boolean combinations. It is equally clear that if the claim holds for some  $\psi$  then it also holds for  $\phi(\bar{x}\bar{y}) = \alpha(\bar{x}\bar{y}) \wedge \neg\psi(\bar{x})$  (note that the guard  $\alpha(\bar{x}\bar{y})$  ensures that the equivalence  $\eta(\psi)(\bar{x}) \leftrightarrow \psi(\bar{x})$  is only ever used for guarded instantiations of  $\bar{x}$ .)

Consider the case of  $\phi = q[\phi_1/U_1, \dots, \phi_s/U_s](\bar{Y}, \bar{x})$  where  $q$  is a UCQ of width  $k$  and each of the  $\phi_i$  is an answer-guarded formula. According to Lemma 4.14,  $\pi : (N, \bar{W}) \xrightarrow{\sim} (M, \pi(\bar{W}))$  is a guarded bisimilar cover allowing for treeifications of width  $k$ . For each  $1 \leq i \leq s$  let  $T_i = \{\bar{b} \mid (N, \bar{W}) \models \eta(\phi_i)(\bar{b})\}$  be the relation defined by  $\eta(\phi_i)$  on  $(N, \bar{W})$ . As  $\phi_i$  is answer-guarded,  $T_i$  is a guarded relation on  $(N, \bar{W})$  hence also on  $N$  and, by guarded-bisimulation invariance of  $\eta(\phi_i)$ , for all guarded tuples  $\bar{b}$  of  $N$  we have  $(N, \bar{W}) \models \eta(\phi_i)(\bar{b}) \iff (M, \pi(\bar{W})) \models \eta(\phi_i)(\pi(\bar{b}))$ . It follows that each  $T_i$  is a  $\pi$ -saturated guarded relation and so, by Lemma 4.14 again,  $\pi : (N, \bar{T}) \xrightarrow{\sim} (M, \pi(\bar{T}))$  is a guarded bisimilar cover allowing for treeifications of width  $k$ . Therefore, as  $q$  has width  $k$ , for every guarded tuple  $\bar{b}$  of  $(N, \bar{T})$  we have that  $(N, \bar{T}) \models q(\bar{b}) \leftrightarrow \Lambda_q^{\tau'}[\eta(\bar{\phi})/\bar{U}](\bar{b})$ , where  $\tau' = \tau \uplus \{U_1, \dots, U_s, C_k\}$ . All in all we have  $(N, \bar{W}) \models q[\eta(\bar{\phi})/\bar{U}](\bar{b}) \leftrightarrow \Lambda_q^{\tau'}[\eta(\bar{\phi})/\bar{U}](\bar{b})$  for all guarded  $\bar{b}$ . Finally, by the induction hypothesis, for each  $\phi_i$  and  $\bar{b}$  a guarded tuple  $(N, \bar{W}) \models \phi_i(\bar{b}) \leftrightarrow \eta(\phi_i)(\bar{b})$ , hence  $(N, \bar{W}) \models \phi(\bar{b}) \leftrightarrow q[\phi/\bar{U}](\bar{b}) \leftrightarrow q[\eta(\bar{\phi})/\bar{U}](\bar{b}) \leftrightarrow \Lambda_q^{\tau'}[\eta(\bar{\phi})/\bar{U}](\bar{b}) \leftrightarrow \eta(\phi)(\bar{b})$ , as needed.

Consider now the case of  $\phi = \mu_{Z, \bar{z}}[\psi(\bar{Y}, Z, \bar{z})]$  and, accordingly,  $\eta(\phi) = [\mu_{Z, \bar{z}}; \eta(\psi)(\bar{Y}, Z, \bar{z})]$ . Let  $(U^\alpha)_\alpha$  and  $(V^\alpha)_\alpha$  be the relations obtained at the respective transfinite stages of the inductive fixpoint computation of  $\psi(\bar{z})$  and by  $\eta(\psi)(\bar{z})$ , respectively. In other words,  $U^0 = V^0 = \emptyset$ ,

$$U^{\alpha+1} = \{\bar{a} \mid (N, \bar{W}, \check{U}^\alpha) \models \psi(\bar{a})\} \quad \text{and} \quad V^{\alpha+1} = \{\bar{a} \mid (N, \bar{W}, \check{V}^\alpha) \models \eta(\psi)(\bar{a})\}$$

for all ordinals  $\alpha$ , moreover,  $U^\lambda = \bigcup_{\alpha < \lambda} U^\alpha$  and  $V^\lambda = \bigcup_{\alpha < \lambda} V^\alpha$  for limit ordinals  $\lambda$ . Here  $\check{U}^\alpha = U^\alpha \cap \text{guarded}(N)$  and  $\check{V}^\alpha = V^\alpha \cap \text{guarded}(N)$  denote the *guarded interior* of  $U^\alpha$  and  $V^\alpha$ , respectively.

Observe that guarded-bisimulation invariance of  $\eta(\psi)$  implies that  $\check{V}^\alpha = \pi^{-1}(\pi(\check{V}^\alpha)) \cap \text{guarded}(N)$  for all ordinals  $\alpha$ . So assuming  $\check{U}^\alpha = \check{V}^\alpha$  for some  $\alpha$ ,  $\check{U}^\alpha$  is  $\pi$ -saturated and thus we can apply the induction hypothesis of the claim of this lemma for the structurally simpler formula  $\psi$  and the assignment mapping  $\bar{Y}$  to  $\bar{W}$  and  $Z$  to  $\check{U}^\alpha$  to establish  $\check{U}^{\alpha+1} = \check{V}^{\alpha+1}$ . Thus it follows by transfinite induction (the limit case being entirely trivial) that  $\check{U}^\alpha = \check{V}^\alpha$  for all ordinals

<sup>3</sup>recall that a guarded relation  $W$  on the cover  $N$  is  $\pi$ -saturated if  $W = \pi^{-1}(\pi(W)) \cap \text{guarded}(N)$

$\alpha$ , whence also  $\bigcup_{\alpha} \check{U}^{\alpha} = \bigcup_{\alpha} \check{V}^{\alpha}$ . In other words, the guarded interiors of the least fixpoints defined by  $\phi$  and by  $\eta(\phi)$  on  $(N, \bar{W})$  do coincide as claimed.  $\square$

**THEOREM 4.17.** *A GNFP<sup>k</sup>-sentence  $\tilde{\varphi}$  in GN-normal form is satisfiable (in the finite) if, and only if,  $\eta(\tilde{\varphi}) \in \text{GFP}^k$  is satisfiable (in the finite).*

**PROOF.** It is easy to see that for every model  $M$  of  $\tilde{\varphi}$  its expansion  $(M, C_k)$  is a model of  $\eta(\tilde{\varphi})$ , where  $C_k$  is the complete  $k$ -ary relation on  $M$ . Indeed, for every positive subformula  $\psi(\bar{x})$  as in (e) above and for every

$$M \models \psi[\phi_1/U_1, \dots, \phi_s/U_s](\bar{a}) \quad (8)$$

there is a CQ  $\exists \bar{y} Q(\bar{x}\bar{y})$ , a disjunct of the CNF of  $\psi$ , such that  $Q$  is a conjunction of  $\{U_1, \dots, U_s\}$ -atoms and  $|\bar{x}| + |\bar{y}| \leq k$  and  $M \models Q[\phi_1/U_1, \dots, \phi_s/U_s](\bar{a}\bar{b})$  for some  $\bar{b} \in M^{|\bar{y}|}$ . Although  $Q$  need not be acyclic  $\Lambda_{\psi}^{\tau\uplus\{U_1, \dots, U_s, C_k\}}(\bar{x})$  does contain as a disjunct the acyclic conjunctive query  $\exists \bar{y} C_k(\bar{x}\bar{y}) \wedge Q(\bar{x}\bar{y})$ . Therefore, given the interpretation of  $C_k$ , we have

$$(M, C_k) \models \Lambda_{\psi}^{\tau\uplus\{U_1, \dots, U_s, C_k\}}[\eta(\phi_1)/U_1, \dots, \eta(\phi_s)/U_s](\bar{a}) \quad (9)$$

and the converse implication (9) $\Rightarrow$ (8) holds by definition of treeification. Using the equivalence of (8) and (9) it is straightforward to verify by induction on formulas that  $(M, C_k) \models \eta(\varphi)(\bar{a})$  iff  $M \models \varphi(\bar{a})$  for all  $\bar{a}$ .

Conversely, consider some  $M$  a model of  $\eta(\tilde{\varphi})$  and its  $(wk^w)$ -th Rosati cover  $M^{(wk^w)}$ , equally a model of  $\eta(\tilde{\varphi})$ , where  $w$  is the maximum of the width of  $\tau$  and  $k$ . Lemma 4.16 proves that  $M^{(wk^w)}$  is, in fact, a model of  $\tilde{\varphi}$ , and we know from Theorem 4.13 that if  $M$  is finite then so is  $M^{(wk^w)}$ .  $\square$

Both satisfiability [Grädel and Walukiewicz 1999] and finite satisfiability [Bárány and Bojańczyk 2012] of GFP sentences have been shown decidable in time  $2^{\mathcal{O}(nw^w)}$ , where  $n$  is the length of the input formula and  $w$  is its width<sup>4</sup>. Starting with a GNFP<sup>k</sup> sentence  $\varphi$  whose GN-normal form is  $\tilde{\varphi}$ , we get from Lemma 4.15 that  $|\eta(\tilde{\varphi})| = 2^{(k|\varphi|)^{\mathcal{O}(1)}}$  and that  $\eta(\tilde{\varphi})$  is computable within that same time bound, but its width remains  $k$ . Theorem 4.4 now follows from these bounds via Theorem 4.17.

## 5. MODEL CHECKING FOR GNFO AND GNFP

In this section we study the combined complexity of the model checking problems for GNFO and GNFP, where the input consists of a sentence and a structure and the goal is to decide whether the sentence is true on the structure. For the *unary negation* cases, it was shown in [ten Cate and Segoufin 2013] that the model checking problem for UNFO is  $\text{P}^{\text{NP}[O(\log^2 n)]}$ -complete, and that the model checking problem for UNFP is in  $\text{NP}^{\text{NP}} \cap \text{coNP}^{\text{NP}}$  and  $\text{P}^{\text{NP}}$ -hard. We show that these upper-bounds also apply to GNFO and GNFP. The proof is a reduction to formulas with unary negations by constructing an incidence structure.

**THEOREM 5.1.** *The model checking problem for GNFO is  $\text{P}^{\text{NP}[O(\log^2 n)]}$ -complete. For GNFP it is in  $\text{NP}^{\text{NP}} \cap \text{coNP}^{\text{NP}}$  and hard for  $\text{P}^{\text{NP}}$ .*

**PROOF.** The lower bounds are immediate as UNFO is a fragment of GNFO and UNFP is a fragment of GNFP. For the upper bounds we reduce the model checking problem for GNFO (resp. GNFP) to the model checking problem for UNFO (resp. UNFP).

Given a relational structure  $M$  and a sentence  $\phi$  of GNFP we construct in polynomial time a relational structure  $M'$  and a sentence  $\phi'$  of UNFP such that  $\phi'$  is in UNFO if  $\phi$  is in GNFO and

$$M \models \phi \text{ iff } M' \models \phi'. \quad (10)$$

<sup>4</sup>The *width* as defined in [Grädel and Walukiewicz 1999; Bárány and Bojańczyk 2012] is the maximal number of free variables occurring in a subformula. This number is of course bounded by the width as defined in this paper.

The structure  $M'$  is an extension of  $M$  essentially representing  $M$  together with its incidence structure.  $M'$  contains one new element per fact of  $M$ . For each relation symbol  $R$  of the signature of  $M$ , we add a new unary symbol  $P_R$  interpreted as the set of all facts of  $M$  involving the relation  $R$ . Finally we add a new binary relation symbol  $E_{R,i}$  for each relation  $R$  of the signature of  $M$  and number  $i$  between 1 and the arity of  $R$ , interpreted as the binary relation that relates each new element  $y$  denoting a fact  $R(\bar{x})$  of  $M$  to  $x_i$ . The construction of  $M'$  is clearly in polynomial time.

When  $\phi$  is in GNFO, the formula  $\phi'$  is constructed from  $\phi$  by first replacing each subformula  $R(\bar{z}) \wedge \neg\psi(\bar{x})$ , where  $\bar{x} \subseteq \bar{z}$  with:

$$\exists y P_R(y) \wedge \bigwedge_i E_{R,i}(y, z_i) \wedge \neg(\exists \bar{x} \bigwedge_i E_{R,\alpha_i}(y, x_i) \wedge \psi(\bar{x}))$$

where  $\alpha_i$  is such that  $x_i = z_{\alpha_i}$ .

In the case where  $\phi$  is in GNFP we further extend the structure constructed above by adding the following for each subformula  $\xi(\bar{z})$  occurring in  $\phi$  and of the form  $\beta(\bar{z}) \wedge Z(\bar{x})$ , where  $Z$  is a fixpoint predicate variable (recall that according to our syntactic restrictions this means  $\bar{x} \subseteq \bar{z}$ ): we have a new unary predicate  $P_\xi$  interpreted with new elements, one per fact of  $M$  in  $\beta$ . Finally, for each  $i$  between 1 and the arity of  $Z$ , we have a new binary relation  $E_{\xi,i}$  interpreted as the pairs  $(v, u_j)$  where  $v$  represents the fact  $\beta(\bar{u})$  and  $j$  is such that  $z_j$  is the variable in position  $i$  within  $Z(\bar{x})$ . This concludes the construction of  $M'$ .

For the construction of  $\phi'$ , we first do as in the GNFO case. Moreover, we have one extra unary fixpoint predicate  $P_z$  per fixpoint predicate  $Z$  occurring in  $\phi$  and we replace each subformula  $\xi(\bar{z})$  of the form  $\beta(\bar{z}) \wedge Z(\bar{x})$  by

$$\exists y P_\xi(y) \wedge P_Z(y) \wedge \bigwedge_i E_{\xi,i}(y, x_i)$$

and each fixpoint subformula  $\mu_{Z,\bar{z}}[\phi(\bar{Y}, Z, \bar{z})](\bar{x})$  by

$$\exists y \mu_{P_Z,z}[\phi(\bar{P}_Y, P_Z, z)](y) \wedge \bigvee_\xi (P_\xi(y) \wedge \bigwedge_i E_{\xi,i}(y, x_i)).$$

In both cases the construction of  $\psi'$  and  $M'$  are clearly in polynomial time. The reader can now verify that (10) holds.  $\square$

*Remark 5.2.* If we had opted for the alternative syntax that does not explicitly declare any concrete guard but instead uses the clause  $\text{guarded}_\tau$  as in (7), then the complexity of the model checking problem would be higher. Indeed it is not difficult to show that in this case it becomes ExpTime-complete. The reason is that if the maximal arity of the relational predicates of the signature is  $k$  then there are exponentially many, in  $k$ , potential guards (in other words predicates  $P_\xi$  in the construction above, accounting for the number of permutations of variables in a  $k$ -ary atom).

With this in mind we encode the model checking problem for a single-rule Datalog program (SIRUP) into the model checking problem of this alternative syntax of GNFP. The former is known to be ExpTime-complete [Gottlob and Papadimitriou 2003]. Given a structure  $M$  and a SIRUP  $\phi$  we introduce a new extra relation whose arity is the number of elements of  $M$  and containing a single tuple that enumerates all elements of  $M$ . The fixpoint formula  $\phi$  is then trivially guarded by this new relation (no need to guard negations because there is no negation in Datalog).

For the upper-bound, given a structure  $M$  and a sentence  $\phi$  of GNFP, we first compute in a new relation, in exponential time, all guarded tuples of  $M$  and then evaluate  $\phi$  as in Theorem 5.1. The total time is exponential, for the algorithm underlying Theorem 5.1 is polynomial in the size of  $M$ .

## 6. EXPRESSIVE POWER OF GNFO AND GNFP

In this section, we develop an appropriate notion of bisimulation for GNFO and GNFP, and use it to characterize the expressive power of GNFO.

Recall the notions of guarded tuples and the notation  $\textit{guarded}(M)$  from Section 2. For a number  $k$ , we say that a tuple is  $k$ -*guarded* if it is guarded by a fact of  $M$  using at most  $k$  elements of  $M$ . We denote by  $\textit{guarded}^k(M)$  the set of all  $k$ -guarded tuples of  $M$ .

*Definition 6.1.* Let  $M, N$  be two structures. A GN-bisimulation (resp. a GN-bisimulation of width  $k \geq 1$ ) is a binary relation  $Z \subseteq \textit{guarded}(M) \times \textit{guarded}(N)$  (resp.  $Z \subseteq \textit{guarded}^k(M) \times \textit{guarded}^k(N)$ ) such that the following hold for every pair  $(\bar{a}, \bar{b}) \in Z$ , where  $\bar{a} = a_1, \dots, a_m$  and  $\bar{b} = b_1, \dots, b_n$

- $(M, \bar{a})$  and  $(N, \bar{b})$  are locally isomorphic (and in particular,  $m = n$ )
- **[Forward clause]** For every finite set  $X \subseteq \textit{dom}(M)$  (resp.  $X \subseteq \textit{dom}(M)$  and  $|X| \leq k$ ) there is a partial homomorphism  $h : M \rightarrow N$  whose domain is  $X$ , such that  $h(a_i) = b_i$  for all  $a_i$  in  $X$ , and such that for every  $\bar{a}' \in \textit{guarded}(M)$  (resp.  $\bar{a}' \in \textit{guarded}^k(M)$ ) consisting of elements in the domain of  $h$ , the pair  $(\bar{a}', h(\bar{a}'))$  belongs to  $Z$ .
- **[Backward clause]** Likewise in the other direction, where  $X \subseteq \textit{dom}(N)$ .

Note that if  $X$  above is restricted to guarded sets then we obtain a definition of guarded bisimulation. We write  $M \approx_{GN} N$  if there is a non-empty GN-bisimulation between  $M$  and  $N$  and write  $M \approx_{GN}^k N$  if the GN-bisimulation has width  $k$ . Notice that  $M \approx_{GN} N$  implies that  $M \approx_{GN}^k N$  for all  $k$ .

It is not difficult to see that the existence of a GN-bisimulation implies indistinguishability by GNFP sentences, and that the existence of a GN-bisimulation of width  $k$  implies indistinguishability in  $\text{GNFP}^k$ .

**PROPOSITION 6.2.** *For  $k \geq 1$ , if  $M \approx_{GN}^k N$  then  $M$  and  $N$  satisfy the same  $\text{GNFP}^k$  sentences. In particular, if  $M \approx_{GN} N$  then  $M$  and  $N$  satisfy the same GNFP sentences.*

**PROOF.** The proof is by induction on the nesting of fixpoints and existential quantification in the formula. We assume without loss of generality that all formulas are in GN-normal form. It is convenient to state the induction hypothesis for formulas  $\phi(\bar{x})$  with several free second-order variables. The induction hypothesis then becomes: for all formulas  $\phi(\bar{x}, \bar{Y})$ , and for all GN-bisimulation  $Z$  of width  $k$  between  $(M, \bar{P})$  and  $(N, \bar{Q})$ , and all pair  $(\bar{a}, \bar{b}) \in Z$ , we have  $(M, \bar{P}, \bar{a}) \models \phi$  iff  $(N, \bar{Q}, \bar{b}) \models \phi$ . We show only the important cases of the inductive step. Let  $M, N$  be two structures,  $Z$  be a GN-bisimulation of width  $k$  between  $M$  and  $N$ ,  $\bar{P}$  and  $\bar{Q}$  be valuations of  $\bar{Y}$  respectively on  $M$  and  $N$ , and  $(\bar{a}, \bar{b}) \in Z$ .

- $\phi(\bar{x}, \bar{Y})$  starts with an existential quantifier. Then, by definition of GN-normal form,  $\phi$  is of the form  $q[\varphi_1/U_1, \dots, \varphi_s/U_s]$  for some UCQ  $q$  and each  $\varphi_i$  is an answer-guarded formula also of the form  $\varphi_i(\bar{y}, \bar{Y})$ . Let  $z_1, \dots, z_n$  be the existentially quantified variables of  $q$  and let  $m = |\bar{x}|$ . In particular  $m + n \leq k$ .

First, suppose  $(M, \bar{P}, \bar{a}) \models \phi$ . Let  $\{c_1, \dots, c_n\}$  be the quantified elements of  $M$  witnessing the truth of  $\phi$  and let  $X = \{c_1, \dots, c_n\} \cup \{a_1, \dots, a_m\}$ . By the definition of GN-bisimulation, there is a partial homomorphism  $h : M \rightarrow N$  of domain  $X$  such that  $h(\bar{a}) = \bar{b}$  and such that  $(\bar{u}, h(\bar{u})) \in Z$  for all  $k$ -guarded tuple  $\bar{u} \subseteq X$ . For each  $i$ , let  $\bar{u}_i$  be the subset of  $X$  making  $\varphi_i$  true on  $(M, \bar{P})$ . As  $\varphi_i$  is answer-guarded and belongs of  $\text{GNFO}^k$ ,  $\bar{u}_i$  is  $k$ -guarded. Therefore, as by induction hypothesis,  $(M, \bar{P}, \bar{u}_i) \models \varphi_i(\bar{y}, \bar{Y})$  iff  $(N, \bar{Q}, h(\bar{u}_i)) \models \varphi_i(\bar{y}, \bar{Y})$ , we have  $(N, \bar{Q}, h(\bar{u}_i)) \models \varphi_i(\bar{y}, \bar{Y})$ . Hence the assignment that sends  $z_1, \dots, z_n$  to  $h(c_1), \dots, h(c_n)$  makes  $\phi$  true on  $(N, \bar{Q}, \bar{b})$ .

The opposite direction, from  $(N, \bar{Q}, \bar{b}) \models \phi$  to  $(M, \bar{P}, \bar{a}) \models \phi$ , is symmetric.

- $\phi(\bar{x}, \bar{Y})$  is any Boolean combination of formulas of the form  $\psi(\bar{y}, \bar{Y})$ , the result is immediate from the induction hypothesis.
- $\phi(\bar{x}, \bar{Y})$  is of the form  $\mu_{Z, \bar{z}}[\psi(Z, \bar{Y}, \bar{z})](\bar{x})$ . We proceed by induction on the fixpoint iterations. Let  $\mathcal{O}_{\psi, (M, \bar{P})}$  and  $\mathcal{O}_{\psi, (N, \bar{Q})}$  be the monotone set-operations induced by  $\psi$  on subsets of the domain of  $(M, \bar{P})$  and  $(N, \bar{Q})$ , respectively, and let  $\kappa = \max\{|M|, |N|\}$ . Recall that the

least fixpoint of  $\mathcal{O}_{\psi, (M, \bar{P})}$  is equal to  $\mathcal{O}_{\psi, (M, \bar{P})}^{\kappa}(\emptyset)$ , and similarly for the least fixpoint of  $\mathcal{O}_{\psi, (N, \bar{Q})}$ . A straightforward transfinite induction shows that, for all ordinals  $\lambda$ , and for all  $(\bar{a}, \bar{b}) \in Z$ ,  $\bar{a} \in \mathcal{O}_{\psi, (M, \bar{P})}^{\lambda}(\emptyset)$  if and only if  $\bar{b} \in \mathcal{O}_{\psi, (N, \bar{Q})}^{\lambda}(\emptyset)$ . We conclude that  $(M, \bar{P}, \bar{a}) \models \mu_{Z, \bar{z}}[\psi(Z, \bar{Y}, \bar{z})](\bar{x})$  if and only if  $(N, \bar{Q}, \bar{b}) \models \mu_{Z, \bar{z}}[\psi(Z, \bar{Y}, \bar{z})](\bar{x})$ .

□

In fact, over arbitrary structures, GN-bisimulation invariance can be used to *characterize* GNFO.

**THEOREM 6.3.** *GNFO is the  $\approx_{GN}$ -invariant fragment of FO, and for all  $k \geq 1$ ,  $\text{GNFO}^k$  is the  $\approx_{GN}^k$ -invariant fragment of FO on arbitrary structures.*

The finite variant of Theorem 6.3, showing that  $\text{GNFO}^k$  captures the  $\approx_{GN}^k$ -invariant fragment of FO on finite structures has recently been established in [Otto 2012].

**PROOF.** We prove the hard direction, which uses the technique of  $\omega$ -saturated structures from classical model theory (cf. [Hodges 1993]). We give the proof for the case of  $\text{GNFO}^k$ . The argument for full GNFO is identical. Let  $\phi$  be any sentence of FO invariant under GN-bisimulations of width  $k$ . We want to show that  $\phi$  is equivalent to a  $\text{GNFO}^k$ -sentence. By a well known argument using Compactness, it is enough to show that, whenever two structures agree on all formulas of  $\text{GNFO}^k$ , they agree on  $\phi$ . Hence, suppose  $M$  and  $N$  satisfy the same sentences of  $\text{GNFO}^k$ . Without loss of generality we can assume that  $M$  and  $N$  are  $\omega$ -saturated. Define  $Z \subseteq \text{guarded}^k(M) \times \text{guarded}^k(N)$  as the set of all  $k$ -guarded pairs  $(\bar{a}, \bar{b})$  such that  $(M, \bar{a})$  and  $(N, \bar{b})$  satisfy the same  $\text{GNFO}^k$ -formulas. We claim that  $Z$  is a non-empty GN-bisimulation of width  $k$ . As  $\phi$  is invariant under GN-bisimulations of width  $k$  this implies that  $M$  and  $N$  agree on  $\phi$  and concludes the proof of the lemma.

That  $Z$  is a GN-bisimulation of width  $k$  follows immediately from the following lemma where we write  $(M, \bar{a}) \equiv_{\text{GNFO}^k} (N, \bar{b})$  (resp.  $(M, \bar{a}) \equiv_{\text{GNFO}} (N, \bar{b})$ ) if for all  $\phi \in \text{GNFO}^k$  (resp.  $\phi \in \text{GNFO}$ ) we have  $M \models \phi(\bar{a})$  iff  $N \models \phi(\bar{b})$ :

**LEMMA 6.4.** *For all  $\omega$ -saturated structures  $M$  and  $N$  the following hold.*

- (1) *The relation  $\{(\bar{a}, \bar{b}) \in \text{guarded}(M) \times \text{guarded}(N) \mid (M, \bar{a}) \equiv_{\text{GNFO}} (N, \bar{b})\}$  is a GN-bisimulation.*
- (2) *The relation  $\{(\bar{a}, \bar{b}) \in \text{guarded}^k(M) \times \text{guarded}^k(N) \mid (M, \bar{a}) \equiv_{\text{GNFO}^k} (N, \bar{b})\}$  is a GN-bisimulation of width  $k$ .*

**PROOF.** We prove the second claim. The proof of the first claim is similar. Let  $Z = \{(\bar{a}, \bar{b}) \in \text{guarded}^k(M) \times \text{guarded}^k(N) \mid (M, \bar{a}) \equiv_{\text{GNFO}^k} (N, \bar{b})\}$ . Clearly,  $Z$  consists of locally isomorphic pairs of tuples. We show that  $Z$  satisfies the forward clause, the proof of the backward clause is analogous.

Suppose  $(\bar{c}, \bar{d}) \in Z$  and let  $X \subseteq \text{dom}(M)$  with  $|X| \leq k$ . For simplicity, assume  $\bar{c} \subseteq X$  (the general case is similar). Thus, let  $X = \{c_1, \dots, c_l, c_{l+1}, \dots, c_n\}$  with  $\bar{c} = (c_1, \dots, c_l)$  and  $n \leq k$ . Let  $T[x_1, \dots, x_n]$  be the set of all formulas  $\phi(x_1, \dots, x_n)$  that are positive Boolean combinations of (i) atomic formulas or (ii) formula of the form  $\alpha(\bar{y}) \wedge \neg\psi(\bar{y})$  where  $\psi$  is in  $\text{GNFO}^k$  and  $\alpha$  is an atomic formula (possibly an equality statement), and that are true in  $(M, c_1, \dots, c_n)$ . We view  $T$  as an  $n$ -type with  $l$  parameters. It is not hard to see that every finite subset  $T' \subseteq T$  is realized in  $N$  under some assignment that sends  $(x_1, \dots, x_l)$  to  $\bar{d}$ . Indeed, notice that  $\exists x_{l+1} \dots x_n (\bigwedge T')$  is a formula of  $\text{GNFO}^k$  true at  $(M, \bar{c})$  and therefore it is also true at  $(N, \bar{d})$  by hypothesis. Since  $N$  is  $\omega$ -saturated (and treating  $T$  as an  $n$ -type with parameter  $\bar{d}$ ), it follows that the entire set  $T[x_1, \dots, x_n]$  is realized in  $N$  under an assignment  $g$  that sends  $(x_1, \dots, x_l)$  to  $\bar{d}$ . Let  $h$  be the mapping sending  $c_i$  to  $g(x_i)$ . As  $T$  contains all atomic formulas, then  $h$  is a homomorphism. Moreover, as  $T$  contains all formula of the form  $\alpha(\bar{y}) \wedge \neg\psi(\bar{y})$ , for all  $\bar{c}'$  in  $\text{guarded}^k(M)$  with  $\bar{c}' \subseteq X$  we have  $(M, \bar{c}') \equiv_{\text{GNFO}^k} (N, h(\bar{c}'))$ . By definition of  $Z$  this implies  $(\bar{c}', h(\bar{c}')) \in Z$ . □

That  $Z$  is non-empty follows from  $\omega$ -saturation: consider  $\bar{a} \in \text{guarded}^k(M)$  and let  $\Sigma(\bar{x})$  be the set of all  $\text{GNFO}^k$  formulas true for  $\bar{a}$ . Every finite subset  $\Sigma' \subseteq \Sigma(\bar{x})$  is realized in  $N$  (notice that  $\exists \bar{x} \bigwedge \Sigma'$  is a sentence of  $\text{GNFO}^k$  that is true in  $M$ , and hence in  $N$ ). Therefore, by  $\omega$ -saturation, the entire set  $\Sigma(\bar{x})$  is realized by an element  $\bar{b}$  in  $N$ , and hence  $(\bar{a}, \bar{b}) \in Z$ , which implies that  $Z$  is non-empty.  $\square$

Based on the definition of GN-bisimulation (of width  $k$ ) it is straightforward to define GN-unraveling (of width  $k$ ) as an operation constructing from any given structure  $M$  a ( $k$ -acyclic) companion  $M^* \equiv_{\text{GNFO}^k} M$ . This provides a natural route for demonstrating the tree-like model property of GNFP. We leave this as an exercise, instead, take a short-cut via the reduction to the guarded fragment introduced in Section 4.

**THEOREM 6.5.** *GNFP has the tree-like model property.*

**PROOF.** Consider a model  $M$  of a  $\text{GNFP}^k$ -sentence  $\varphi$ . Recall Section 4 and the reduction from GNFP to GFP. We can assume without loss of generality that  $M$  contains the relation  $C_k$  containing all  $k$  tuples on  $M$ . In this case  $M$  is also a model for  $\eta(\varphi)$ , where  $\eta(\varphi)$  is the GFP formula constructed in section 4. Let  $M^*$  be the guarded unraveling of  $M$  of width  $k$  (cf. e.g. [Grädel 1999a] for the relevant definitions). It is straightforward to verify that  $M^*$  is a  $k$ -guarded bisimilar cover of  $M$ , that  $M^*$  has tree width at most  $k$ , and that  $M^*$  is acyclic (in particular, weakly  $l$ -acyclic as a cover of  $M$  for every  $l \in \mathbb{N}$ ). Therefore, by Lemma 4.16 we have  $M^* \models \eta(\varphi)$  iff  $M^* \models \varphi$ . By guarded bisimulation we also have  $M^* \models \eta(\varphi)$  iff  $M \models \eta(\varphi)$ . Altogether this shows that  $M^* \models \varphi$ .  $\square$

## 7. FURTHER EXTENSIONS

### 7.1. Clique-Guarded Negation

We now consider a further generalization of GNFO called CGNFP, taking inspiration from the clique-guarded fragment. CGNFP is defined just like GNFP except that we allow clique-guards in the place of guards. We say that a conjunction of atomic formulas  $\alpha$  *clique-guards*  $\bar{x}$  if for every pair  $x_i, x_j \in \bar{x}$ ,  $\alpha$  includes a conjunct in which both  $x_i$  and  $x_j$  appear (in other words, the co-occurrence graph for the variables in  $\bar{x}$  is a clique).

The formulas of CGNFP are generated by the following grammar:

$$\begin{aligned} \phi ::= & R(\bar{x}) \mid x=y \mid \alpha(\bar{x}, \bar{y}) \wedge X(\bar{x}) \mid \phi_1 \wedge \phi_2 \mid \phi_1 \vee \phi_2 \mid \exists x \phi \mid \alpha(\bar{x}, \bar{y}) \wedge \neg \phi(\bar{x}) \mid \\ & \mu_{Z, \bar{z}}[\phi(\bar{Y}, Z, \bar{z})](\bar{x}) \end{aligned}$$

where  $\alpha(\bar{x}, \bar{y})$  is a conjunction of atoms that clique-guards  $\bar{x}$ . The fixpoint-free fragment of CGNFP is called CGNFO, and we use the notation  $\text{CGNFP}[\tau]$  or  $\text{CGNFO}[\tau]$  when restricting to formulas in a particular signature  $\tau$ . As in the case of GNFO and GNFP, in the above inductive definition, we can equivalently replace the clauses for conjunction, disjunction and existential quantification by a single clause for unions of conjunctive queries. As in the case of GNFP this provides a normal form that is used to define formulas of width  $k$ , denoted  $\text{CGNFP}^k$ .

In this section, we show that CGNFO and CGNFP behave similarly to GNFO and GNFP, in terms of the complexity of satisfiability, and in terms of the finite model property. To prove this, we will make use the fact that the  $n$ -th Rosati cover  $M^{(n)}$  of a structure  $M$  is  $n$ -conformal (cf. Theorem 4.13). Recall that we call a structure  $M$   $n$ -conformal (where  $n \geq 1$ ) if every  $n$ -tuple that is clique-guarded in  $M$  is in fact guarded in  $M$ . Using this fact, it turns out that our results for GNFO and GNFP can be lifted to CGNFO and CGNFP without much effort.

**THEOREM 7.1.**

- (1) *The satisfiability problem for CGNFO and for CGNFP is 2ExpTime-complete.*
- (2) *CGNFO has the finite model property.*

Theorem 7.1 generalizes prior decidability results for the *loosely guarded fragment* [van Benthem 1997], the *packed fragment* [Marx 1999], and the *clique-guarded fragment* [Grädel 1999a], which

are all subsumed in CGNFO (for sentences). The finite model property for these fragments was first established in [Hodkinson 2002].

In the remainder of this section, we explain how Theorem 7.1 is proved.

We extend our translation from GNFP into GFP to a translation from CGNFP into GFP. With a slight abuse of notation, we use the same symbol  $\eta$  also to denote this extension of the translation. For every  $k \geq 1$ , and for every relational signature  $\tau$  consisting of at most  $k$ -ary relations, we define a translation  $\eta$  from  $\text{CGNFP}^k[\tau]$  formulas in normal form to  $\text{GFP}^k[\tau \uplus \{C_k\}]$  formulas, where  $C_k$  is a new symbol of arity  $k$ , by structural recursion, using the following rules.

$$\begin{aligned} \eta(R(\bar{x})) &= R(\bar{x}) & (a) \\ \eta(\alpha(\bar{x}\bar{y}) \wedge Z(\bar{x})) &= \alpha(\bar{x}\bar{y}) \wedge Z(\bar{x}) & (b) \\ \eta(\alpha(\bar{x}\bar{y}) \wedge \neg\psi(\bar{x})) &= \alpha(\bar{x}\bar{y}) \wedge \neg\eta(\psi(\bar{x})) & (c) \\ \eta(\mu_{Z,\bar{z}}[\psi(\bar{Y}, Z, \bar{z})]) &= \mu_{Z,\bar{z}}[\eta(\psi(\bar{Y}, Z, \bar{z}))] & (d) \\ \eta(q[\phi_1/U_1, \dots, \phi_s/U_s]) &= \Lambda_q^{\tau \uplus \{U_1, \dots, U_s, C_k\}}[\eta(\phi_1)/U_1, \dots, \eta(\phi_s)/U_s] & (e) \end{aligned}$$

where in (e)  $q$  is a UCQ of signature  $\{U_1, \dots, U_s\}$  disjoint from  $\tau \uplus \{\bar{Y}, C_k\}$  and  $\phi_1, \dots, \phi_s \in \text{GNFP}^k[\tau \uplus \{\bar{Y}\}]$ , where  $\bar{Y}$  enumerates the free fixpoint variables occurring in any of the  $\phi_i$ 's, each  $\phi_i$  being a answer-clique-guarded formula, and such that  $q[\phi_1/U_1, \dots, \phi_s/U_s]$  is a subformula of  $\tilde{\varphi}$ .

Recall Theorem 4.17, which states that the translation  $\eta(\cdot)$  from GNFP to GFP is satisfiability preserving. The proof involved passing from a structure  $M$  to its  $(wk^w)$ -th Rosati cover  $M^{(wk^w)}$ , which is  $(wk^w)$ -acyclic, and applying Lemma 4.16. Lemma 4.16, in turn, was proved by induction, where the inductive hypothesis was stated in terms of guarded tuples and guarded relations. Using the  $(wk^w)$ -conformality of  $M^{(wk^w)}$ , which gives us that every clique-guarded  $(wk^w)$ -tuple is in fact a guarded tuple, the same arguments apply for clique guarded tuples and therefore when the input is in CGNFP. In this way, we get the following analogue of Theorem 4.17.

**THEOREM 7.2.** *A  $\text{CGNFP}^k$ -formula  $\tilde{\varphi}$  in normal form is satisfiable (in the finite) if, and only if, the  $\text{GFP}^k$ -formula  $\eta(\tilde{\varphi})$  is satisfiable (in the finite).*

Moreover, the same complexity analysis applies as in the case of GNFP. In particular, Theorem 7.2 implies that satisfiability is 2Exp-complete for CGNFP. Furthermore, observe that the translation  $\eta$  maps CGNFO formulas to GFO formulas. Therefore, Theorem 7.2 also establishes the finite model property for CGNFO.

## 7.2. Constant Symbols

Although our definition of GNFO, and of GNFP, does not include constant symbols, they can be added without affecting any of our complexity results. This can be shown using the same technique that was used in [Grädel 1999b] in the context of the guarded fragment. For the sake of completeness, we explain here how this technique can be applied to CGNFP-sentences (the same argument works also for CGNFP-formulas with free variables).

By a *CGNFP-sentence with constants* we mean a CGNFP-formula where, in addition, constant symbols may freely be used in atomic subformulas (and there is no restriction on the use of constant symbols in negated subformulas).

**PROPOSITION 7.3.** *Given any CGNFP-sentence  $\phi$  with constant symbols, we can construct in polynomial time a CGNFP-sentence  $\phi'$  without constant symbols, such that  $\phi$  and  $\phi'$  are equisatisfiable, both in the finite and over arbitrary structures.*

**PROOF.** Let  $\phi$  be any CGNFP-sentence over a signature  $\sigma = \{R_1, \dots, R_n, c_1, \dots, c_k\}$ . Consider the relational signature  $\tau = \{R'_1, \dots, R'_n\}$ , where the arity of each new relation symbol  $R'_i$  is the arity of  $R_i$  plus  $k$ . Fix fresh variables  $z_1, \dots, z_k$  corresponding to the constants  $c_1, \dots, c_k$ .

Finally, let  $\phi^*(z_1, \dots, z_k)$  be the CGNFP-formula over  $\tau$  obtained from  $\phi$  by (i) replacing every occurrence of a constant symbol  $c_i$  by the corresponding variable  $z_i$ , and, subsequently, (ii) replacing every relational atomic formula  $R_j(x_1, \dots, x_m)$  by  $R_j(x_1, \dots, x_m, z_1, \dots, z_k)$ . Note that  $\phi^*(z_1, \dots, z_k)$  is indeed a CGNFP-formula. This follows from the fact that  $\phi$  was a CGNFP-formula, and the fact  $z_1, \dots, z_k$  occur in every atomic subformula of  $\phi^*(z_1, \dots, z_k)$ .

We show that  $\phi$  and  $\phi^*(z_1, \dots, z_k)$  are equi-satisfiable, both in the finite and in the infinite.

Indeed, every model  $M$  of  $\phi$  gives rise to a structure  $M'$  over the same domain and such that for each relation symbol  $R_i \in \sigma$  we have  $R_i^{M'} = R_i^M \times \{c_1^M\} \times \dots \times \{c_k^M\}$ . It is then immediate to check that  $M' \models \phi^*(c_1^M, \dots, c_k^M)$ .

Conversely, if  $M' \models \phi^*(u_1, \dots, u_k)$  for some  $u_1, \dots, u_k \in \text{dom}(M')$ , then  $M \models \phi$ , where, for each  $m$ -ary relation symbol  $R_i$ ,  $R_i^M = \{(a_1, \dots, a_m) \mid (a_1, \dots, a_m, u_1, \dots, u_k) \in R_i^{M'}\}$  and where  $c_j^M = u_j$ .

Finally, we can turn  $\phi^*$  into a sentence by existentially quantifying out  $z_1, \dots, z_k$ .  $\square$

The same argument also applies to the model checking problem (as the construction of the model  $M'$  from  $M$  given in the above proof is polynomial).

## 8. DISCUSSION

We have provided a logical framework generalizing both GFO and UNFO while preserving their nice properties, in particular decidability of satisfiability. Our results on satisfiability carry over to the validity and entailment problems for GNFO, and likewise for GNFP, as these problems are all reducible to each other. For instance, a GNFO entailment  $\phi(\bar{x}\bar{y}) \models \psi(\bar{x}\bar{z})$  holds if, and only if, for a fresh relation  $R$  of appropriate arity  $\exists \bar{x}\bar{y}\bar{z}(\phi(\bar{x}\bar{y}) \wedge R(\bar{x}\bar{y}\bar{z}) \wedge \neg\psi(\bar{x}\bar{z}))$  is not satisfiable.

Another immediate consequence of our results is that query answering for unions of conjunctive queries with respect to guarded-negation fixpoint theories (i.e., the analogue of Theorem 3.3 replacing GFO by GNFP) is decidable and 2ExpTime-complete.

It would be tempting to further generalize by including the two variable fragment of FO (FO<sup>2</sup>). Unfortunately this would lead to undecidability. Actually a simple combination of FO<sup>2</sup> with UNFO already yields undecidability as FO<sup>2</sup> can express the fact that a relation correspond to inequality (by  $\forall x, y (R(x, y) \leftrightarrow x \neq y)$ ) and the extension of UNFO with inequality [ten Cate and Segoufin 2013]. Similarly, unconstrained universal quantification leads to undecidability, since every subformula of the form  $\neg\psi(\bar{x})$  can be trivially guarded using a fresh relation  $R(\bar{x})$ , adding  $\forall \bar{x} R\bar{x}$  as a conjunct to the main formula.

Since the publication of the conference proceedings version of the present paper, a number of new results and applications of guarded-negation logics have been established. In particular, in [Bárány et al. 2012], it was shown that boundedness is decidable for guarded-negation datalog; in [Bárány et al. 2013], GNFO was shown to satisfy Craig interpolation as well as various model-theoretic preservation theorems; and in [Bárány et al. 2013] and [Bienvenu et al. 2013], open-world query answering and query rewritability were studied for database queries and constraints specified in GNFO.

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