# The Complexity of Second-order HyperLTL\*

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#### Abstract

We determine the complexity of second-order HyperLTL satisfiability, finite-state satisfiability, and model-checking: All three are as hard as truth in third-order arithmetic.

We also consider two fragments of second-order HyperLTL that have been introduced with the aim to facilitate effective model-checking by restricting the sets one can quantify over. The first one restricts second-order quantification to smallest/largest sets that satisfy a guard while the second one restricts second-order quantification further to least fixed points of (first-order) HyperLTL definable functions.

The first fragment is still as hard as truth in third-order arithmetic while satisfiability for the second one is  $\Sigma_1^1$ -complete, i.e., only as hard as (first-order) HyperLTL and therefore much less complex. Finally, finite-state satisfiability and model-checking are in  $\Sigma_2^2$  and  $\Sigma_1^1$ -hard, and thus also less complex than model-checking full second-order HyperLTL.

#### 1 Introduction

The introduction of hyperlogics [5] for the specification and verification of hyperproperties [6] – properties that relate multiple system executions, has been one of the major success stories of formal verification during the last decade. Logics like HyperLTL and HyperCTL<sup>\*</sup>, the extensions of LTL [16] and CTL<sup>\*</sup> [7] (respectively) with trace quantification, are natural specification languages for information-flow and security properties, have a decidable model-checking problem [9], and hence found many applications in program verification.

However, while expressive enough to express common information-flow properties, they are unable to express other important hyperproperties, e.g., common knowledge in multi-agent systems and asynchronous hyperproperties (witnessed by a plethora of asynchronous extensions of HyperLTL, e.g., [1, 4, 13]). These examples all have in common that they are *second-order* properties, i.e., they naturally require quantification over *sets* of traces, while HyperLTL (and HyperCTL<sup>\*</sup>) only allows quantification over traces.

In light of this situation, Beutner et al. [2] introduced the logic Hyper<sup>2</sup>LTL, which extends HyperLTL with second-order quantification, i.e., quantification over sets of traces. They show that the logic is indeed able to capture common knowledge, asynchronous extensions of HyperLTL, and many other applications. However, they also note that this expressiveness comes at a steep price: model-checking Hyper<sup>2</sup>LTL is highly undecidable, i.e.,  $\Sigma_1^1$ -hard. Thus, their main result is a partial model-checking algorithm for a fragment of Hyper<sup>2</sup>LTL where second-order quantification degenerates to least fixed point computations of HyperLTL definable functions. Their algorithm over- and underapproximates these fixed points and then invokes a HyperLTL model-checking algorithm on these approximations. A prototype implementation of the algorithm is able to model-check properties capturing common knowledge, asynchronous hyperproperties, and distributed computing. In a recent work [3], Beutner et al. also suggest a monitoring algorithm for this fixed point fragment.

However, one question has been left open: Just how complex is Hyper<sup>2</sup>LTL verification?

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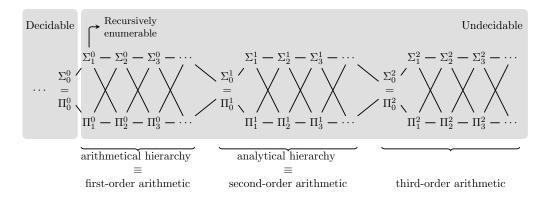


Figure 1: The arithmetical hierarchy, the analytical hierarchy, and beyond.

**Complexity Classes for Undecidable Problems.** The complexity of undecidable problems is typically captured in terms of the arithmetical and analytical hierarchy, where decision problems (encoded as subsets of  $\mathbb{N}$ ) are classified based on their definability by formulas of higher-order arithmetic, namely by the type of objects one can quantify over and by the number of alternations of such quantifiers. We refer to Roger's textbook [18] for fully formal definitions and refer to Figure 1 for a visualization.

The class  $\Sigma_1^0$  contains the sets of natural numbers of the form

$$\{x \in \mathbb{N} \mid \exists x_0. \cdots \exists x_k. \ \psi(x, x_0, \dots, x_k)\}$$

where quantifiers range over natural numbers and  $\psi$  is a quantifier-free arithmetic formula. Note that this is exactly the class of recursively enumerable sets. The notation  $\Sigma_1^0$  signifies that there is a single block of existential quantifiers (the subscript 1) ranging over natural numbers (type 0 objects, explaining the superscript 0). Analogously,  $\Sigma_1^1$  is induced by arithmetic formulas with existential quantification of type 1 objects (sets of natural numbers) and arbitrary (universal and existential) quantification of type 0 objects. So,  $\Sigma_1^0$  is part of the first level of the arithmetical hierarchy while  $\Sigma_1^1$  is part of the first level of the analytical hierarchy. In general, level  $\Sigma_n^0$  (level  $\Pi_n^0$ ) of the arithmetical hierarchy is induced by formulas with at most n alternations between existential and universal type 0 quantifiers, starting with an existential (universal) quantifier. Similar hierarchies can be defined for arithmetic of any fixed order by limiting the alternations of the highest-order quantifiers and allowing arbitrary lower-order quantification. In this work, the highest order we are concerned with is three, i.e., quantification over sets of sets of natural numbers.

HyperLTL satisfiability is  $\Sigma_1^1$ -complete [11], HyperLTL finite-state satisfiability is  $\Sigma_1^0$ -complete [8, 12], and, as mentioned above, Hyper<sup>2</sup>LTL model-checking is  $\Sigma_1^1$ -hard [2], but, prior to this current work, no upper bounds were known for Hyper<sup>2</sup>LTL.

Another yardstick is truth for order k arithmetic, i.e., the question whether a given sentence of order k arithmetic evaluates to true. In the following, we are in particular interested in the case k = 3, i.e., we consider formulas with arbitrary quantification over type 0 objects, type 1 objects, and type 2 objects (sets of sets of natural numbers). Note that these formulas span the whole third hierarchy, as we allow arbitrary nesting of existential and universal third-order quantification.

**Our Contributions.** In this work, we determine the exact complexity of Hyper<sup>2</sup>LTL satisfiability and model-checking, as well as some variants of satisfiability, for the full logic and the two fragments introduced by Beutner et al., as well as for two variations of the semantics.

An important stepping stone for us is the investigation of the cardinality of models of Hyper<sup>2</sup>LTL. It is known that every satisfiable HyperLTL sentence has a countable model, and that some have no finite models [10]. This restricts the order of arithmetic that can be simulated in HyperLTL and explains in particular the  $\Sigma_1^1$ -completeness of HyperLTL satisfiability [11]. We show that (unsurprisingly) second-order quantification allows to write formulas that only have uncountable models by generalizing the lower bound construction of HyperLTL to Hyper<sup>2</sup>LTL. Note that the cardinality of the continuum is a trivial upper bound on the size of models, as they are sets of traces.

With this tool at hand, we are able to show that Hyper<sup>2</sup>LTL satisfiability is as hard as truth in third-order arithmetic, i.e., much harder than HyperLTL satisfiability. This in itself is not surprising, as second-order quantification can be expected to increase the complexity considerably. But what might be surprising at first glance is that the problem is not  $\Sigma_1^2$ -complete, i.e., at the same position of the third hierarchy that HyperLTL satisfiability occupies in one full hierarchy below (see Figure 1). However, arbitrary second-order trace quantification corresponds to arbitrary quantification over type 2 objects, which allows to capture the full third hierarchy.

Furthermore, we also show that Hyper<sup>2</sup>LTL finite-state satisfiability is as hard as truth in third-order arithmetic, and therefore as hard as general satisfiability. This should be contrasted with the situation for HyperLTL described above, where finite-state satisfiability is  $\Sigma_1^0$ -complete (i.e., recursively enumerable) and thus much simpler than general satisfiability, which is  $\Sigma_1^1$ -complete.

Finally, our techniques for Hyper<sup>2</sup>LTL satisfiability also shed light on the complexity of Hyper<sup>2</sup>LTL model-checking, which we show to be as hard as truth in third-order arithmetic as well, i.e., all three problems we consider have the same complexity. In particular, this increases the lower bound on Hyper<sup>2</sup>LTL model-checking from  $\Sigma_1^1$  to truth in third-order arithmetic. Again, this has be contrasted with the situation for HyperLTL, where model-checking is decidable, albeit TOWER-complete [17, 15].

So, quantification over arbitrary sets of traces makes verification very hard. However, Beutner et al. noticed that many of the applications of Hyper<sup>2</sup>LTL described above do not require full second-order quantification, but can be expressed with restricted forms of second-order quantification. To capture this, they first restrict second-order quantification to smallest/largest sets satisfying a guard (obtaining the fragment Hyper<sup>2</sup>LTL<sub>fp</sub>) and then further restrict those to least fixed points induced by HyperLTL definable operators (obtaining the fragment lfp-Hyper<sup>2</sup>LTL<sub>fp</sub>). By construction, these least fixed points are unique, i.e., second-order quantification degenerates to least fixed point computation.

Nevertheless, we show that  $Hyper^2LTL_{fp}$  retains the same complexity as  $Hyper^2LTL$ , i.e., all three problems are still as hard as truth in third-order arithmetic: Just restricting to guarded second-order quantification does not decrease the complexity. For all results mentioned so far, it is irrelevant whether we allow second-order quantifiers to range over sets of traces that may contain traces that are not in the model (standard semantics) or whether we restrict these quantifiers to subsets of the model (closed-world semantics). But if we consider lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> satisfiability under closed-world semantics, the complexity finally decreases to  $\Sigma_1^1$ -completeness. Stated differently, one can add least fixed points of HyperLTL definable operators to HyperLTL without increasing the complexity of the satisfiability problem.

Finally, for lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> finite-state satisfiability and model-checking, we prove  $\Sigma_2^2$ -membership and  $\Sigma_1^1$  lower bounds for both semantics, thereby confining the complexity to the second level of the third hierarchy.

Table 1 lists our results and compares them to LTL and HyperLTL. Recall that Beutner et al. showed that lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> yields (partial) model checking and monitoring algorithms [2, 3]. Our results confirm the usability of the lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> fragment also from a theoretical point of view, as all problems relevant for verification have significantly lower complexity (albeit, still highly undecidable).

All formal proofs are omitted due to space restrictions and can be found in the appendix.

#### 2 Preliminaries

We denote the nonnegative integers by  $\mathbb{N}$ . An alphabet is a nonempty finite set. The set of infinite words over an alphabet  $\Sigma$  is denoted by  $\Sigma^{\omega}$ . Throughout this paper, we fix a finite set AP of atomic propositions. A trace over AP is an infinite word over the alphabet  $2^{AP}$ .

A transition system  $\mathfrak{T} = (V, E, I, \lambda)$  consists of a finite set V of vertices, a set  $E \subseteq V \times V$  of (directed) edges, a set  $I \subseteq V$  of initial vertices, and a labeling  $\lambda \colon V \to 2^{AP}$  of the vertices by sets of atomic propositions. We assume that every vertex has at least one outgoing edge. A path  $\rho$  through  $\mathfrak{T}$  is an infinite

Table 1: List of our results (in bold) and comparison to related logics. "T3OA-complete" stands for "as hard as truth in third-order arithmetic". Entries marked with an asterisk only hold for closed-world semantics, all others hold for both semantics.

Logic	Satisfiability	Finite-state satisfiability	Model-checking
LTL	PSpace-complete	PSpace-complete	PSpace-complete
HyperLTL	$\Sigma_1^1$ -complete	$\Sigma_1^0$ -complete	Tower-complete
Hyper <sup>2</sup> LTL	T3OA-complete	T3OA-complete	T3OA-complete
$\mathrm{Hyper}^{2}\mathrm{LTL}_{fp}$	T3OA-complete	T3OA-complete	T3OA-complete
$lfp-Hyper^{2}LTL_{fp}$	$\Sigma_1^1 ext{-complete}^*$	$\Sigma_1^1$ -hard/in $\Sigma_2^2$	$\Sigma_1^1$ -hard/in $\Sigma_2^2$

sequence  $\rho(0)\rho(1)\rho(2)\cdots$  of vertices with  $\rho(0) \in I$  and  $(\rho(n), \rho(n+1)) \in E$  for every  $n \ge 0$ . The trace of  $\rho$  is defined as  $\lambda(\rho) = \lambda(\rho(0))\lambda(\rho(1))\lambda(\rho(2))\cdots$ . The set of traces of  $\mathfrak{T}$  is  $\operatorname{Tr}(\mathfrak{T}) = \{\lambda(\rho) \mid \rho \text{ is a path through } \mathfrak{T}\}.$ 

#### 2.1 Hyper<sup>2</sup>LTL

Let  $\mathcal{V}_1$  be a set of first-order trace variables (i.e., ranging over traces) and  $\mathcal{V}_2$  be a set of second-order trace variables (i.e., ranging over sets of traces) such that  $\mathcal{V}_1 \cap \mathcal{V}_2 = \emptyset$ . We typically use  $\pi$  (possibly with decorations) to denote first-order variables and X, Y, Z (possibly with decorations) to denote second-order variables. Also, we assume the existence of two distinguished second-order variables  $X_a, X_d \in \mathcal{V}_2$  such that  $X_a$  refers to the set  $(2^{AP})^{\omega}$  of all traces, and  $X_d$  refers to the universe of discourse (the set of traces the formula is evaluated over).

The formulas of Hyper<sup>2</sup>LTL are given by the grammar

$$\begin{split} \varphi &::= \exists X. \ \varphi \mid \forall X. \ \varphi \mid \exists \pi \in X. \ \varphi \mid \forall \pi \in X. \ \varphi \mid \psi \\ \psi &::= \mathbf{p}_{\pi} \mid \neg \psi \mid \psi \lor \psi \mid \mathbf{X} \ \psi \mid \psi \ \mathbf{U} \ \psi \end{split}$$

where **p** ranges over AP,  $\pi$  ranges over  $\mathcal{V}_1$ , X ranges over  $\mathcal{V}_2$ , and **X** (next) and **U** (until) are temporal operators. Conjunction ( $\wedge$ ), exclusive disjunction ( $\oplus$ ), implication ( $\rightarrow$ ), and equivalence ( $\leftrightarrow$ ) are defined as usual, and the temporal operators eventually (**F**) and always (**G**) are derived as  $\mathbf{F}\psi = \neg\psi \mathbf{U}\psi$  and  $\mathbf{G}\psi = \neg \mathbf{F} \neg \psi$ .

A sentence is a formula without free (first- and second-order) variables, which are defined as usual. We measure the size of a formula by its number of distinct subformulas.

The semantics of Hyper<sup>2</sup>LTL is defined with respect to a variable assignment, a partial mapping  $\Pi: \mathcal{V}_1 \cup \mathcal{V}_2 \to (2^{AP})^{\omega} \cup 2^{(2^{AP})^{\omega}}$  such that

- if  $\Pi(\pi)$  for  $\pi \in \mathcal{V}_1$  is defined, then  $\Pi(\pi) \in (2^{AP})^{\omega}$  and
- if  $\Pi(X)$  for  $X \in \mathcal{V}_2$  is defined, then  $\Pi(X) \in 2^{(2^{AP})^{\omega}}$ .

Given a variable assignment  $\Pi$ , a variable  $\pi \in \mathcal{V}_1$ , and a trace t, we denote by  $\Pi[\pi \mapsto t]$  the assignment that coincides with  $\Pi$  on all variables but  $\pi$ , which is mapped to t. Similarly, given a variable assignment  $\Pi$ , a variable  $X \in \mathcal{V}_2$ , and a set T of traces we denote by  $\Pi[X \mapsto T]$  the assignment that coincides with  $\Pi$ everywhere but X, which is mapped to T. Furthermore,  $\Pi[j, \infty)$  denotes the variable assignment mapping every  $\pi \in \mathcal{V}_1$  in  $\Pi$ 's domain to  $\Pi(\pi)(j)\Pi(\pi)(j+1)\Pi(\pi)(j+2)\cdots$ , the suffix of  $\Pi(\pi)$  starting at position j(the assignment of variables  $X \in \mathcal{V}_2$  is not updated, as this is not necessary for our application).

For a variable assignment  $\Pi$  we define

- $\Pi \models p_{\pi}$  if  $p \in \Pi(\pi)(0)$ ,
- $\Pi \models \neg \psi$  if  $\Pi \not\models \psi$ ,
- $\Pi \models \psi_1 \lor \psi_2$  if  $\Pi \models \psi_1$  or  $\Pi \models \psi_2$ ,

- $\Pi \models \mathbf{X} \psi$  if  $\Pi[1, \infty) \models \psi$ ,
- $\Pi \models \psi_1 \mathbf{U} \psi_2$  if there is a  $j \ge 0$  such that  $\Pi[j, \infty) \models \psi_2$  and for all  $0 \le j' < j$  we have  $\Pi[j', \infty) \models \psi_1$ ,
- $\Pi \models \exists \pi \in X. \varphi$  if there exists a trace  $t \in \Pi(X)$  such that  $\Pi[\pi \mapsto t] \models \varphi$ ,
- $\Pi \models \forall \pi \in X. \ \varphi$  if for all traces  $t \in \Pi(X)$  we have  $\Pi[\pi \mapsto t] \models \varphi$ ,
- $\Pi \models \exists X. \varphi$  if there exists a set  $T \subseteq (2^{AP})^{\omega}$  such that  $\Pi[X \mapsto T] \models \varphi$ , and
- $\Pi \models \forall X. \varphi$  if for all sets  $T \subseteq (2^{AP})^{\omega}$  we have  $\Pi[X \mapsto T] \models \varphi$ .

The variable assignment with empty domain is denoted by  $\Pi_{\emptyset}$ . We say that a set T of traces satisfies a Hyper<sup>2</sup>LTL sentence  $\varphi$ , written  $T \models \varphi$ , if  $\Pi_{\emptyset}[X_a \mapsto (2^{AP})^{\omega}, X_d \mapsto T] \models \varphi$ , i.e., if we assign the set of all traces to  $X_a$  and the set T to the universe of discourse  $X_d$ . In this case, we say that T is a model of  $\varphi$ . A transition system  $\mathfrak{T}$  satisfies  $\varphi$ , written  $\mathfrak{T} \models \varphi$ , if  $\operatorname{Tr}(\mathfrak{T}) \models \varphi$ . Slightly sloppily, we again say that  $\mathfrak{T}$  satisfies  $\varphi$  in this case. Although Hyper<sup>2</sup>LTL sentences are required to be in prenex normal form, HyperLTL sentences are closed under Boolean combinations, which can easily be seen by transforming such a sentence into an equivalent one in prenex normal form (which might require renaming of variables). Thus, in examples and proofs we will often use Boolean combinations of Hyper<sup>2</sup>LTL sentences.

**Remark 1.** HyperLTL is the fragment of Hyper<sup>2</sup>LTL obtained by disallowing second-order quantification and only allowing first-order quantification of the form  $\exists \pi \in X_d$  and  $\forall \pi \in X_d$ , i.e., one can only quantify over traces from the universe of discourse. Hence, we typically simplify our notation to  $\exists \pi$  and  $\forall \pi$  in HyperLTL formulas.

#### 2.2 Closed-World Semantics

Let us highlight that second-order quantification in Hyper<sup>2</sup>LTL as defined by Beutner et al. [2] (and introduced above) ranges over arbitrary sets of traces (not necessarily from the universe of discourse) and that first-order quantification ranges over elements in such sets, i.e., (possibly) again over arbitrary traces. To disallow this, we introduce *closed-world* semantics for Hyper<sup>2</sup>LTL. Here, we only consider formulas that do not use the variable  $X_a$  and change the semantics of the set quantifiers as follows:

- $\Pi \models_{\mathrm{cw}} \exists X. \varphi$  if there exists a set  $T \subseteq \Pi(X_d)$  such that  $\Pi[X \mapsto T] \models \varphi$ , and
- $\Pi \models_{\mathrm{cw}} \forall X. \varphi$  if for all sets  $T \subseteq \Pi(X_d)$  we have  $\Pi[X \mapsto T] \models \varphi$ .

The closed-world semantics of atomic propositions, Boolean connectives, and temporal operators is defined as before.

We say that  $T \subseteq (2^{AP})^{\omega}$  satisfies  $\varphi$  under closed-world semantics, if  $\Pi_{\emptyset}[X_d \mapsto T] \models_{cw} \varphi$ . Hence, under closed-world semantics, second-order quantifiers only range over subsets of the universe of discourse. Consequently, first-order quantifiers also range over traces from the universe of discourse.

**Lemma 1.** Every Hyper<sup>2</sup>LTL sentence  $\varphi$  can in polynomial time be translated into a Hyper<sup>2</sup>LTL sentence  $\varphi'$  such that for all sets T of traces we have  $T \models_{cw} \varphi$  if and only if  $T \models \varphi'$  (under standard semantics).

Thus, all complexity upper bounds we derive in this paper for standard semantics also hold for closedworld semantics and all lower bounds for closed-world semantics also hold for standard semantics.

#### 2.3 Arithmetic

We consider formulas of arithmetic, i.e., predicate logic with signature  $(+, \cdot, <, \in)$ , evaluated over the structure  $(\mathbb{N}, +, \cdot, <, \in)$ . A type 0 object is a natural number in  $\mathbb{N}$ , a type 1 object is a subset of  $\mathbb{N}$ , and a type 2 object is a set of subsets of  $\mathbb{N}$ . Our benchmark is third-order arithmetic, i.e., predicate logic with quantification over type 0, type 1, and type 2 objects. In the following, we use lower-case roman letters (possibly with decorations) for first-order variables, upper-case roman letters (possibly with decorations) for second-order variables, and upper-case calligraphic roman letters (possibly with decorations) for third-order variables. Note that every fixed natural number is definable in first-order arithmetic, so we freely use them as syntactic sugar. Truth of third-order arithmetic is the following decision problem: given a sentence  $\varphi$  of third-order arithmetic, does  $(\mathbb{N}, +, \cdot, <, \in)$  satisfy  $\varphi$ ?

Arithmetic formulas with a single free first-order variable define sets of natural numbers. We are interested in the classes

- $\Sigma_1^1$  containing sets of the form  $\{x \in \mathbb{N} \mid \exists X_1 \subseteq \mathbb{N}. \dots \exists X_k \subseteq \mathbb{N}. \psi(x, X_1, \dots, X_k)\}$ , where  $\psi$  is a formula of arithmetic with arbitrary quantification over type 0 objects (but no second-order quantifiers), and
- $\Sigma_2^2$  containing sets of the form

$$\{x \in \mathbb{N} \mid \exists \mathcal{X}_1 \subseteq 2^{\mathbb{N}}. \cdots \exists \mathcal{X}_k \subseteq 2^{\mathbb{N}}. \forall \mathcal{Y}_1 \subseteq 2^{\mathbb{N}}. \cdots \forall \mathcal{Y}_{k'} \subseteq 2^{\mathbb{N}}. \psi(x, \mathcal{X}_1, \dots, \mathcal{X}_k, \mathcal{Y}_1, \dots, \mathcal{Y}_{k'})\},\$$

where  $\psi$  is a formula of arithmetic with arbitrary quantification over type 0 and type 1 objects (but no third-order quantifiers).

# 3 The Cardinality of Hyper<sup>2</sup>LTL Models

A Hyper<sup>2</sup>LTL sentence is satisfiable if it has a model. In this section, we investigate the cardinality of models of satisfiable Hyper<sup>2</sup>LTL sentences. We begin by stating a (trivial) upper bound, which follows from the fact that models are sets of traces. Here,  $\mathfrak{c}$  denotes the cardinality of the continuum (equivalently, the cardinality of  $2^{\mathbb{N}}$  and of  $(2^{\mathbb{AP}})^{\omega}$  for any finite nonempty set AP).

**Proposition 1.** Every satisfiable  $Hyper^2LTL$  sentence has a model of cardinality at most  $\mathfrak{c}$ .

In this section, we show that this trivial upper bound is tight.

**Remark 2.** There is a very simple, albeit equally unsatisfactory, way to obtain the desired lower bound: Consider  $\forall \pi \in X_a$ .  $\exists \pi' \in X_d$ .  $\mathbf{G} \bigwedge_{p \in \mathrm{AP}} p_{\pi} \leftrightarrow p_{\pi'}$  expressing that every trace in the set of all traces is also in the universe of discourse, i.e.,  $(2^{\mathrm{AP}})^{\omega}$  is its only model. However, this crucially relies on the fact that  $X_a$  is, by definition, interpreted as the set of all traces. In fact, the formula does not even use second-order quantification.

We show how to construct a sentence that has only uncountable models, and which retains that property under closed-world semantics (which in particular means it cannot use  $X_a$ ). This should be compared with HyperLTL, where every satisfiable sentence has a countable model [10]: Unsurprisingly, the addition of (even closed-world) second-order quantification increases the cardinality of minimal models, even without cheating.

There is a HyperLTL sentence that requires every natural number to be encoded by a distinct trace in its unique model [10]. Thus, we present a Hyper<sup>2</sup>LTL sentence that requires every *set* of natural numbers to be encoded by a distinct trace in its unique model.

**Theorem 1.** There is a satisfiable  $X_a$ -free Hyper<sup>2</sup>LTL sentence that only has models of cardinality  $\mathfrak{c}$  (both under standard and closed-world semantics).

# 4 The Complexity of Hyper<sup>2</sup>LTL Satisfiability

The Hyper<sup>2</sup>LTL satisfiability problem asks, given a Hyper<sup>2</sup>LTL sentence  $\varphi$ , whether  $\varphi$  is satisfiable. In this section, we determine tight bounds on the complexity of the Hyper<sup>2</sup>LTL satisfiability problem and some of its variants.

The proof of Theorem 1 relies on constructing a sentence that requires each of its models to encode every subset of  $\mathbb{N}$  by a trace in the model. Hence, sets of traces can encode sets of sets of natural numbers,

i.e., type 2 objects. Another important ingredient is the implementation of addition and multiplication in HyperLTL following Fortin et al. [12]. Combining both, we show that Hyper<sup>2</sup>LTL and truth in third-order arithmetic have the same complexity.

**Theorem 2.** The Hyper<sup>2</sup>LTL satisfiability problem is polynomial-time equivalent to truth in third-order arithmetic. The lower bound holds even for  $X_a$ -free sentences.

Again, let us also consider the lower bound under closed-world semantics.

**Corollary 1.** The  $Hyper^2LTL$  satisfiability problem under closed-world semantics is polynomial-time equivalent to truth in third-order arithmetic.

The Hyper<sup>2</sup>LTL finite-state satisfiability problem asks, given a Hyper<sup>2</sup>LTL sentence  $\varphi$ , whether there is a finite transition system satisfying  $\varphi$ . Note that we do not ask for a finite set T of traces satisfying  $\varphi$ . In fact, the set of traces of the finite transition system may still be infinite or even uncountable. Nevertheless, the problem is potentially simpler, as there are only countably many finite transition systems (and their sets of traces are much simpler). However, we show that the finite-state satisfiability problem is as hard as the general satisfiability problem, as Hyper<sup>2</sup>LTL allows the quantification over arbitrary (sets of) traces, i.e., restricting the universe of discourse to the traces of a finite transition system does not restrict secondorder quantification at all (as the set of all traces is represented by a finite transition system). This has to be contrasted with the finite-state satisfiability problem for HyperLTL (defined analogously), which is  $\Sigma_1^0$ -complete (a.k.a. recursively enumerable), as HyperLTL model-checking of finite transition systems is decidable [5].

**Theorem 3.** The Hyper<sup>2</sup>LTL finite-state satisfiability problem is polynomial-time equivalent to truth in third-order arithmetic. The lower bound holds even for  $X_a$ -free sentences.

Again, let us also consider the case of closed-world semantics.

**Corollary 2.** The Hyper<sup>2</sup>LTL finite-state satisfiability problem under closed-world semantics is polynomialtime equivalent to truth in third-order arithmetic.

# 5 The Complexity of Hyper<sup>2</sup>LTL Model-Checking

The Hyper<sup>2</sup>LTL model-checking problem asks, given a finite transition system  $\mathfrak{T}$  and a Hyper<sup>2</sup>LTL sentence  $\varphi$ , whether  $\mathfrak{T} \models \varphi$ . Beutner et al. [2] have shown that Hyper<sup>2</sup>LTL model-checking is  $\Sigma_1^1$ -hard, but there is no known upper bound in the literature. We improve the lower bound considerably, i.e., also to truth in third-order arithmetic, and then show that this bound is tight. This is the first upper bound on the problem's complexity.

**Theorem 4.** The Hyper<sup>2</sup>LTL model-checking problem is polynomial-time equivalent to truth in third-order arithmetic. The lower bound already holds for  $X_a$ -free sentences.

Again, the lower bound proof can easily be extended to closed-world semantics.

**Corollary 3.** The  $Hyper^2LTL$  model-checking problem under closed-world semantics is polynomial-time equivalent to truth in third-order arithmetic.

# 6 Hyper<sup>2</sup>LTL<sub>fp</sub>

As we have seen, unrestricted second-order quantification makes  $Hyper^2LTL$  very expressive and therefore highly undecidable. But restricted forms of second-order quantification are sufficient for many application areas. Hence, Beutner et al. [2] introduced  $Hyper^2LTL_{fp}$ , a fragment of  $Hyper^2LTL$  in which secondorder quantification ranges over smallest/largest sets that satisfy a given guard. For example, the formula  $\exists (X, \Upsilon, \varphi_1). \varphi_2$  expresses that there is a set T of traces that satisfies both  $\varphi_1$  and  $\varphi_2$ , and T is a smallest set that satisfies  $\varphi_1$  (i.e.,  $\varphi_1$  is the guard). This fragment is expressive enough to express common knowledge, asynchronous hyperproperties, and causality in reactive systems [2].

The formulas of  $Hyper^2LTL_{fp}$  are given by the grammar

$$\varphi ::= \exists (X, \mathfrak{K}, \varphi). \varphi \mid \forall (X, \mathfrak{K}, \varphi). \varphi \mid \exists \pi \in X. \varphi \mid \forall \pi \in X. \varphi \mid \psi$$
$$\psi ::= \mathbf{p}_{\pi} \mid \neg \psi \mid \psi \lor \psi \mid \mathbf{X} \psi \mid \psi \mathbf{U} \psi$$

where **p** ranges over AP,  $\pi$  ranges over  $\mathcal{V}_1$ , X ranges over  $\mathcal{V}_2$ , and  $\mathfrak{X} \in \{\Upsilon, \lambda\}$ , i.e., the only modification concerns the syntax of second-order quantification.

Accordingly, the semantics of Hyper<sup>2</sup>LTL<sub>fp</sub> is similar to that of Hyper<sup>2</sup>LTL but for the second-order quantifiers, for which we define (for  $\mathfrak{X} \in \{\Upsilon, \Lambda\}$ ):

- $\Pi \models \exists (X, \mathfrak{X}, \varphi_1). \varphi_2$  if there exists a set  $T \in \operatorname{sol}(\Pi, (X, \mathfrak{X}, \varphi_1))$  such that  $\Pi[X \mapsto T] \models \varphi_2$ , and
- $\Pi \models \forall (X, \mathfrak{X}, \varphi_1). \varphi_2$  if for all sets  $T \in \mathrm{sol}(\Pi, (X, \mathfrak{X}, \varphi_1))$  we have  $\Pi[X \mapsto T] \models \varphi_2$ ,

where sol( $\Pi$ ,  $(X, \mathfrak{X}, \varphi_1)$ ) is the set of all minimal/maximal models of the formula  $\varphi_1$ , which is defined as follows:

$$\operatorname{sol}(\Pi, (X, \Upsilon, \varphi_1)) = \{T \subseteq (2^{\operatorname{AP}})^{\omega} \mid \Pi[X \mapsto T] \models \varphi_1 \text{ and } \Pi[X \mapsto T'] \not\models \varphi_1 \text{ for all } T' \subsetneq T\}$$
$$\operatorname{sol}(\Pi, (X, \lambda, \varphi_1)) = \{T \subseteq (2^{\operatorname{AP}})^{\omega} \mid \Pi[X \mapsto T] \models \varphi_1 \text{ and } \Pi[X \mapsto T'] \not\models \varphi_1 \text{ for all } T' \supsetneq T\}$$

Note that  $sol(\Pi, (X, \mathfrak{X}, \varphi_1))$  may be empty or may contain multiple sets, which then are pairwise incomparable.

Let us also define closed-world semantics for  $\text{Hyper}^2 \text{LTL}_{fp}$ . Here, we again disallow the use of the variable  $X_a$  and change the semantics of set quantification to

- $\Pi \models_{\mathrm{cw}} \exists (X, \mathfrak{X}, \varphi_1). \varphi_2$  if there exists a set  $T \in \mathrm{sol}_{\mathrm{cw}}(\Pi, (X, \mathfrak{X}, \varphi_1))$  such that  $\Pi[X \mapsto T] \models \varphi_2$ , and
- $\Pi \models_{\mathrm{cw}} \forall (X, \mathfrak{X}, \varphi_1). \varphi_2$  if for all sets  $T \in \mathrm{sol}_{\mathrm{cw}}(\Pi, (X, \mathfrak{X}, \varphi_1))$  we have  $\Pi[X \mapsto T] \models \varphi_2$ ,

where

$$\operatorname{sol}_{\operatorname{cw}}(\Pi, (X, \curlyvee, \varphi_1)) = \{T \subseteq \Pi(X_d) \mid \Pi[X \mapsto T] \models_{\operatorname{cw}} \varphi_1$$
  
and  $\Pi[X \mapsto T'] \not\models_{\operatorname{cw}} \varphi_1$  for all  $T' \subsetneq T\}$   
$$\operatorname{sol}_{\operatorname{cw}}(\Pi, (X, \land, \varphi_1)) = \{T \subseteq \Pi(X_d) \mid \Pi[X \mapsto T] \models_{\operatorname{cw}} \varphi_1$$
  
and  $\Pi[X \mapsto T'] \not\models_{\operatorname{cw}} \varphi_1$  for all  $T' \supseteq T\}.$ 

Note that  $\operatorname{sol}_{\operatorname{cw}}(\Pi, (X, \mathfrak{X}, \varphi_1))$  may still be empty or may contain multiple sets, but all sets are now incomparable subsets of  $\Pi(X_d)$ .

A Hyper<sup>2</sup>LTL<sub>fp</sub> formula is a sentence if it does not have any free variables (also in the guards). Models are defined as for Hyper<sup>2</sup>LTL.

**Proposition 2** (Proposition 1 of [2]). Every  $Hyper^2LTL_{fp}$  sentence  $\varphi$  can in polynomial time be translated into a  $Hyper^2LTL$  sentence  $\varphi'$  such that for all sets T of traces we have  $T \models \varphi$  if and only if  $T \models \varphi'$ .<sup>1</sup>

The same claim is also true for closed-world semantics, which can be proven using the same proof.

**Remark 3.** Every  $Hyper^2 LTL_{fp}$  sentence  $\varphi$  can in polynomial time be translated into a  $Hyper^2 LTL$  sentence  $\varphi'$  such that for all sets T of traces we have  $T \models_{cw} \varphi$  if and only if  $T \models_{cw} \varphi'$ .

 $<sup>^{1}</sup>$ The polynomial-time claim is not made in [2], but follows from the construction when using appropriate data structures for formulas.

Thus, every complexity upper bound for Hyper<sup>2</sup>LTL also holds for Hyper<sup>2</sup>LTL<sub>fp</sub> and every lower bound for Hyper<sup>2</sup>LTL<sub>fp</sub> also holds for Hyper<sup>2</sup>LTL. In the following, we show that lower bounds can also be transferred in the other direction, i.e., from Hyper<sup>2</sup>LTL to Hyper<sup>2</sup>LTL<sub>fp</sub>. Thus, contrary to the design goal of Hyper<sup>2</sup>LTL<sub>fp</sub>, it is in general not more feasible than full Hyper<sup>2</sup>LTL.

We begin again by studying the cardinality of models of  $\text{Hyper}^2 \text{LTL}_{fp}$  sentences, which will be the key technical tool for our complexity results. Again, as such formulas are evaluated over sets of traces, whose cardinality is bounded by  $\mathfrak{c}$ , there is a trivial upper bound. Our main result is that this bound is tight even for the restricted setting of  $\text{Hyper}^2 \text{LTL}_{fp}$ .

**Theorem 5.** There is a satisfiable  $X_a$ -free  $Hyper^2LTL_{fp}$  sentence that only has models of cardinality c (under standard and closed-world semantics).

Now, let us describe how we settle the complexity of  $\text{Hyper}^2\text{LTL}_{fp}$  satisfiability and model-checking: Recall that  $\text{Hyper}^2\text{LTL}$  allows set quantification over arbitrary sets of traces while  $\text{Hyper}^2\text{LTL}_{fp}$  restricts quantification to minimal/maximal sets of traces that satisfy a guard formula. By using a sentence  $\varphi_{\mathfrak{c}}$  as guard that has only models of cardinality  $\mathfrak{c}$ , the minimal sets satisfying the guard have cardinality  $\mathfrak{c}$ . Thus, we can obtain every possible set over propositions not used by  $\varphi_{\mathfrak{c}}$  as a minimal set satisfying the guard.

**Theorem 6.**  $Hyper^2 LTL_{fp}$  satisfiability, finite-state satisfiability, and model-checking are polynomial-time equivalent to truth in third-order arithmetic. The lower bound holds even for  $X_a$ -free sentences.

Let us conclude by mentioning that Theorem 5 and Theorem 6 can again be generalized to  $\text{Hyper}^2 \text{LTL}_{fp}$ under closed-world semantics, using the same arguments as for full  $\text{Hyper}^2 \text{LTL}$ .

**Corollary 4.**  $Hyper^2 LTL_{fp}$  satisfiability, finite-state satisfiability, and model-checking under closed-world semantics are polynomial-time equivalent to truth in third-order arithmetic.

# 7 The Least Fixed Point Fragment of $Hyper^2 LTL_{fp}$

We have seen that even restricting second-order quantification to smallest/largest sets that satisfy a guard formula is essentially as expressive as full Hyper<sup>2</sup>LTL. However, Beutner et al. note that applications like common knowledge and asynchronous hyperproperties do not even require quantification over smallest/largest sets satisfying a guard, they "only" require quantification over least fixed points of HyperLTL definable functions [2]. This finally yields a fragment with (considerably) lower complexity: satisfiability under closedworld semantics is  $\Sigma_1^1$ -complete while finite-state satisfiability and model-checking are in  $\Sigma_2^2$  and  $\Sigma_1^1$ -hard (under both semantics). For satisfiability under closed-world semantics, this matches the complexity of HyperLTL satisfiability.

Recall that a  $Hyper^2 LTL_{fp}$  sentence using only minimality constraints has the form

$$\varphi = \gamma_1. \ Q_1(Y_1, \Upsilon, \varphi_1^{\text{con}}). \ \gamma_2. \ Q_2(Y_2, \Upsilon, \varphi_2^{\text{con}}). \ \dots \gamma_k. \ Q_k(Y_k, \Upsilon, \varphi_k^{\text{con}}). \ \gamma_{k+1}\psi$$

satisfying the following properties:

- Each  $\gamma_j$  is a block  $\gamma_j = Q_{\ell_{j-1}+1} \pi_{\ell_{j-1}+1} \in X_{\ell_{j-1}+1} \cdots Q_{\ell_j} \pi_{\ell_j} \in X_{\ell_j}$  of trace quantifiers (with  $\ell_0 = 0$ ). As  $\varphi$  is a sentence, this implies that we have  $\{X_{\ell_j+1}, \ldots, X_{\ell_{j+1}}\} \subseteq \{X_a, X_d, Y_1, \ldots, Y_{j-1}\}$ .
- $\psi$  is a quantifier-free formula. Again, as  $\varphi$  is a sentence, the free variables of  $\psi$  are among the trace variables quantified in the  $\gamma_j$ .

Now,  $\varphi$  is an lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> sentence<sup>2</sup>, if additionally

<sup>&</sup>lt;sup>2</sup>Our definition here differs slightly from the one in [2] in that we require the existence of some traces in the fixed point (via the subformulas  $\dot{\pi}_1 \triangleright Y_j$ ). Without these, the least fixed point would always be the empty set. All examples and applications of [2] are also of this form.

• each  $\varphi_i^{\text{con}}$  has the form

$$\varphi_j^{\mathrm{con}} = \dot{\pi}_1 \triangleright Y_j \land \dots \land \dot{\pi}_n \triangleright Y_j \land \forall \ddot{\pi}_1 \in Z_1. \ \dots \forall \ddot{\pi}_{n'} \in Z_{n'}. \ \psi_j^{\mathrm{step}} \to \ddot{\pi}_m \triangleright Y_j$$

for some  $n, n' \ge 1$ , where

 $\begin{aligned} &-\{\dot{\pi}_1,\ldots,\dot{\pi}_n\} \subseteq \{\pi_0,\ldots,\pi_{\ell_j}\},\\ &-\{Z_1,\ldots,Z_{n'}\} \subseteq \{X_a,X_d,Y_0,\ldots,Y_j\},\\ &-\psi_j^{\text{step}} \text{ is a quantifier-free formula whose free variables are among } \ddot{\pi}_1,\ldots,\ddot{\pi}_{n'},\pi_1,\ldots,\pi_{\ell_j}, \text{ and}\\ &-1 \leq m \leq n'. \end{aligned}$ 

Here, we use  $\pi \triangleright X$  as shorthand for  $\exists \pi' \in X$ .  $\mathbf{G} \bigwedge_{\mathbf{p} \in AP} \mathbf{p}_{\pi} \leftrightarrow \mathbf{p}_{\pi'}$ , which expresses that the trace  $\pi$  is in the set X of traces. As always,  $\varphi_j^{\text{con}}$  can be brought into the required prenex normal form.

Let us give some intuition for the definition. To this end, fix some  $j \in \{1, 2, ..., k\}$  and a variable assignment  $\Pi$  whose domain contains at least all variables quantified before  $Y_j$ , i.e., all  $Y_{j'}$  and all variables in the  $\gamma_{j'}$  for j' < j, as well as  $X_a$  and  $X_d$ . Then,

$$\varphi_j^{\mathrm{con}} = \dot{\pi}_1 \in Y_j \land \dots \land \dot{\pi}_n \in Y_j \land \left( \forall \ddot{\pi}_1 \in Z_1. \dots \forall \ddot{\pi}_{n'} \in Z_{n'}. \psi_j^{\mathrm{step}} \to \ddot{\pi}_m \triangleright Y_j \right)$$

induces the monotonic function  $f_{\Pi,j} \colon 2^{(2^{AP})^{\omega}} \to 2^{(2^{AP})^{\omega}}$  defined as

$$f_{\Pi,j}(S) = \{\Pi(\dot{\pi}_1), \dots, \Pi(\dot{\pi}_n)\} \cup \{\Pi'(\ddot{\pi}_m) \mid \Pi' = \Pi[\ddot{\pi}_1 \mapsto t_1, \dots, \ddot{\pi}_{n'} \mapsto t_{n'}]$$
  
for  $t_i \in \Pi(Z_i)$  if  $Z_i \neq Y_i$  and  $t_i \in S$  if  $Z_i = Y_i$  s.t.  $\Pi' \models \psi_i^{\text{step}}\}.$ 

We define  $S_0 = \emptyset$ ,  $S_{\ell+1} = f_{\Pi,j}(S_\ell)$ , and  $\operatorname{lfp}(\Pi, j) = \bigcup_{\ell \in \mathbb{N}} S_\ell$ , which is the least fixed point of  $f_{\Pi,j}$ . Due to the minimality constraint on  $X_j$  in  $\varphi$ ,  $\operatorname{lfp}(\Pi, j)$  is the unique set in  $\operatorname{sol}(\Pi, (Y_j, \Upsilon, \varphi_j^{\operatorname{con}}))$ . Hence, an induction shows that  $\operatorname{lfp}(\Pi, j)$  only depends on the values  $\Pi(\pi)$  for trace variables  $\pi$  quantified before  $Y_j$  as well as the values  $\Pi(X_d)$  and  $\Pi(X_a)$ , but not on the values  $\Pi(Y_{j'})$  for j' < j.

Thus, as  $sol(\Pi, (Y_j, \Upsilon, \varphi_j^{con}))$  is a singleton, it is irrelevant whether  $Q_j$  is an existential or a universal quantifier. Instead of interpreting second-order quantification as existential or universal, here one should understand it as a deterministic least fixed point computation: choices for the trace variables and the two distinguished second-order variables uniquely determine the set of traces that a second-order quantifier assigns to a second-order variable.

**Remark 4.** Note that the traces that are added to a fixed point assigned to  $Y_j$  either come from another  $Y_{j'}$  with j' < j, from the model (via  $X_d$ ) or from the set of all traces (via  $X_a$ ). Thus, for  $X_a$ -free formulas, all second-order quantifiers range over (unique) subsets of the model, i.e., there is no point in an explicit definition of closed-world semantics. The analogue of closed-world semantics for lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> is just to restrict oneself to  $X_a$ -free sentences.

In the remainder of this section, we study the complexity of lfp-Hyper<sup>2</sup>LTL<sub>fp</sub>. For the satisfiability result, the key step is again to study the size of models of satisfiable sentences. For lfp-Hyper<sup>2</sup>LTL<sub>fp</sub>, as for HyperLTL, we are able to show that each satisfiable sentence without  $X_a$  has a countable model. The following result is proven by generalizing the proof for the analogous result for HyperLTL [10]: we show that every model T of a sentence  $\varphi$  without  $X_a$  contains a countable  $R \subseteq T$  that is closed under the application of Skolem functions and the functions  $f_{\Pi,j}$  for suitable variable assignments  $\Pi$ . This allows us to show that R is also a model of  $\varphi$ .

**Lemma 2.** Every satisfiable  $X_a$ -free lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> sentence has a countable model.

Before we continue with our complexity results, let us briefly mention that the formula from Remark 2 shows that the restriction to  $X_a$ -free sentences is essential to obtain the upper bound above.

With this upper bound, we can express the existence of (w.l.o.g.) countable models of a given sentence  $\varphi$  via arithmetic formulas that only use existential quantification of type 1 objects (sets of natural numbers), which are rich enough to express countable sets T of traces and objects (e.g., Skolem functions and more) witnessing that T satisfies  $\varphi$ . This places satisfiability in  $\Sigma_1^1$  while the matching lower bound already holds for HyperLTL [11].

**Theorem 7.** Lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> satisfiability for  $X_a$ -free sentences is  $\Sigma_1^1$ -complete.

Finally, we consider finite-state satisfiability and model-checking. Note that we have to deal with uncountable sets of traces in both problems, as the sets of traces of finite transition systems may be uncountable.

**Theorem 8.** Lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> finite-state satisfiability and model-checking are both in  $\Sigma_2^2$  and  $\Sigma_1^1$ -hard, where the lower bound already holds for  $X_a$ -free sentences.

#### 8 Conclusion

We have investigated and settled the complexity of satisfiability, finite-state satisfiability, and model-checking for Hyper<sup>2</sup>LTL and Hyper<sup>2</sup>LTL<sub>fp</sub> and (almost) settled it for lfp-Hyper<sup>2</sup>LTL<sub>fp</sub>. For the former two, all three problems are as hard as truth in third-order arithmetic, and therefore (not surprisingly) much harder than the corresponding problems for HyperLTL, which are "only"  $\Sigma_1^1$ -complete,  $\Sigma_1^0$ -complete, and TOWERcomplete, respectively. This shows that the addition of second-order quantification increases the already high complexity of HyperLTL significantly. However, for the fragment lfp-Hyper<sup>2</sup>LTL<sub>fp</sub>, in which second-order quantification degenerates to least fixed point computations, the complexity is much lower: satisfiability under closed-world semantics is  $\Sigma_1^1$ -complete and finite-state satisfiability as well as model-checking are in  $\Sigma_2^2$ .

In future work, we aim to answer several questions raised by this work:

- Our complexity results for Hyper<sup>2</sup>LTL<sub>fp</sub> only use maximality constraints, i.e., second-order quantifiers range over largest sets satisfying the guards. What is the complexity of Hyper<sup>2</sup>LTL<sub>fp</sub> with minimality constraints only?
- Our complexity result for  $lfp-Hyper^2LTL_{fp}$  satisfiability pertains to closed-world semantics. What is the complexity of  $lfp-Hyper^2LTL_{fp}$  satisfiability under standard semantics?
- There is a gap in our complexity results for lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> finite-state satisfiability and modelchecking, i.e., they are Σ<sup>1</sup><sub>1</sub>-hard and in Σ<sup>2</sup><sub>2</sub>. What is the complexity of lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> finite-state satisfiability and model-checking?
- Just as one can (as we have done here) study lfp-Hyper<sup>2</sup>LTL<sub>fp</sub>, one can also consider gfp-Hyper<sup>2</sup>LTL<sub>fp</sub> where set quantifiers range over greatest fixed points. What is the complexity of gfp-Hyper<sup>2</sup>LTL<sub>fp</sub>?
- Similar to the standard vs. closed world semantics for Hyper<sup>2</sup>LTL, the logic HyperQPTL [17] extends HyperLTL by quantification over atomic propositions, or, in our language, by quantification over arbitrary traces. What is the complexity of HyperQPTL?

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## Appendix

In this appendix, we present the proofs omitted in the main part. Throughout, we use the following shorthands to simplify our formulas:

- Given  $AP' \subseteq AP$ , the AP'-projection of a trace  $t(0)t(1)t(2)\cdots$  over AP is the trace  $(t(0) \cap AP')(t(1) \cap AP')(t(2) \cap AP')\cdots$  over AP'.
- We write  $\pi =_{AP'} \pi'$  for a set  $AP' \subseteq AP$  for the formula  $\mathbf{G} \bigwedge_{\mathbf{p} \in AP'} (\mathbf{p}_{\pi} \leftrightarrow \mathbf{p}_{\pi'})$  expressing that the AP'-projection of  $\pi$  and the AP'-projection of  $\pi'$  are equal.
- As already introduced in Section 7 of the main part, we write  $\pi \triangleright X$  for the formula  $\exists \pi' \in X$ .  $\pi =_{AP} \pi'$  expressing that the trace  $\pi$  is in X.

## A Proof of Lemma 1

Recall that we need to show that every Hyper<sup>2</sup>LTL sentence  $\varphi$  can in polynomial time be translated into a Hyper<sup>2</sup>LTL sentence  $\varphi'$  such that for all sets T of traces we have  $T \models_{cw} \varphi$  if and only if  $T \models \varphi'$  (under standard semantics).

*Proof.* Second-order quantification over subsets of the universe of discourse can easily be mimicked by guarding classical quantifiers ranging over arbitrary sets. Here, we rely on the formula

$$\psi_{\subseteq X_d}(X) = \forall \pi \in X. \ \exists \pi' \in X_d. \ \pi =_{\mathrm{AP}} \pi',$$

which expresses that every trace in X is also in  $X_d$ .

Now, given a Hyper<sup>2</sup>LTL sentence  $\varphi$ , let  $\varphi'$  be the Hyper<sup>2</sup>LTL sentence obtained by recursively replacing

- each existential second-order quantifier  $\exists X. \ \psi \text{ in } \varphi \text{ by } \exists X. \ \psi_{\subset X_d}(X) \land \psi$ ,
- each universal second-order quantifier  $\forall X. \ \psi \text{ in } \varphi \text{ by } \forall X. \ \psi_{\subset X_d}(X) \to \psi$ ,

and then bringing the resulting sentence into prenex normal form, which can be done as no quantifier is under the scope of a temporal operator.  $\hfill \Box$ 

## **B** Proof of Theorem 1

Recall that we need to show that there is a satisfiable  $X_a$ -free Hyper<sup>2</sup>LTL sentence that only has models of cardinality  $\mathfrak{c}$  (both under standard and closed-world semantics).

**Example 1.** We begin by recalling a construction of Finkbeiner and Zimmermann giving a satisfiable Hyper-LTL sentence  $\psi$  that has no finite models [10]. The sentence intuitively posits the existence of a unique trace for every natural number n. Our lower bound for Hyper<sup>2</sup>LTL builds upon that construction.

Fix  $AP = \{x\}$  and consider the conjunction  $\psi = \psi_1 \wedge \psi_2 \wedge \psi_3$  of the following three formulas:

- 1.  $\psi_1 = \forall \pi. \neg \mathbf{x}_{\pi} \mathbf{U}(\mathbf{x}_{\pi} \land \mathbf{X} \mathbf{G} \neg \mathbf{x}_{\pi})$ : every trace in a model is of the form  $\emptyset^n \{\mathbf{x}\} \emptyset^{\omega}$  for some  $n \in \mathbb{N}$ , i.e., every model is a subset of  $\{\emptyset^n \{\mathbf{x}\} \emptyset^{\omega} \mid n \in \mathbb{N}\}$ .
- 2.  $\psi_2 = \exists \pi. \mathbf{x}_{\pi}$ : the trace  $\emptyset^0 \{\mathbf{x}\} \emptyset^{\omega}$  is in every model.
- 3.  $\psi_3 = \forall \pi$ .  $\exists \pi'$ .  $\mathbf{F}(\mathbf{x}_{\pi} \wedge \mathbf{X} \mathbf{x}_{\pi'})$ : if  $\emptyset^n \{\mathbf{x}\} \emptyset^{\omega}$  is in a model for some  $n \in \mathbb{N}$ , then also  $\emptyset^{n+1} \{\mathbf{x}\} \emptyset^{\omega}$ .

Then,  $\psi$  has exactly one model (over AP), namely  $\{\emptyset^n \{ x \} \emptyset^\omega \mid n \in \mathbb{N} \}$ .

Traces of the form  $\emptyset^n \{\mathbf{x}\} \emptyset^{\omega}$  indeed encode natural numbers and  $\psi$  expresses that every model contains the encodings of all natural numbers and nothing else. But we can of course also encode sets of natural numbers with traces as follows: a trace t over a set of atomic propositions containing  $\mathbf{x}$  encodes the set  $\{n \in \mathbb{N} \mid \mathbf{x} \in t(n)\}$ . In the following, we show that second-order quantification allows us to express the existence of the encodings of all subsets of natural numbers by requiring that for every subset  $S \subseteq \mathbb{N}$  (quantified as the set  $\{\emptyset^n \{\mathbf{x}\} \emptyset^{\omega} \mid n \in S\}$  of traces) there is a trace t encoding S, which means  $\mathbf{x}$  is in t(n) if and only if S contains a trace in which  $\mathbf{x}$  holds at position n. This equivalence can be expressed in Hyper<sup>2</sup>LTL. For technical reasons, we do not capture the equivalence directly but instead use encodings of both the natural numbers that are in S and the natural numbers that are not in S.

*Proof.* We first prove that there is a satisfiable  $X_a$ -free Hyper<sup>2</sup>LTL sentence  $\varphi_{allSets}$  whose unique model (under standard semantics) has cardinality  $\mathfrak{c}$ . To this end, we fix AP = {+, -, s, x} and consider the conjunction  $\varphi_{allSets} = \varphi_0 \wedge \cdots \wedge \varphi_4$  of the following formulas:

- $\varphi_0 = \forall \pi \in X_d$ .  $\bigvee_{\mathbf{p} \in \{+,-,\mathbf{s}\}} \mathbf{G}(\mathbf{p}_{\pi} \land \bigwedge_{\mathbf{p}' \in \{+,-,\mathbf{s}\} \setminus \{\mathbf{p}\}} \neg \mathbf{p}'_{\pi})$ : In each trace of a model, one of the propositions in  $\{+,-,\mathbf{s}\}$  holds at every position and the other two propositions in  $\{+,-,\mathbf{s}\}$  hold at none of the positions. Consequently, we speak in the following about type  $\mathbf{p}$  traces for  $\mathbf{p} \in \{+,-,\mathbf{s}\}$ .
- $\varphi_1 = \forall \pi \in X_d$ .  $(+_{\pi} \lor -_{\pi}) \to \neg \mathbf{x}_{\pi} \mathbf{U}(\mathbf{x}_{\pi} \land \mathbf{X} \mathbf{G} \neg \mathbf{x}_{\pi})$ : Type **p** traces for  $\mathbf{p} \in \{+, -\}$  in the model have the form  $\{\mathbf{p}\}^n \{\mathbf{x}, \mathbf{p}\} \{\mathbf{p}\}^{\omega}$  for some  $n \in \mathbb{N}$ .
- $\varphi_2 = \bigwedge_{p \in \{+,-\}} \exists \pi \in X_d$ .  $p_{\pi} \land x_{\pi}$ : for both  $p \in \{+,-\}$ , the type p trace  $\{p\}^0 \{x,p\} \{p\}^{\omega}$  is in every model.
- $\varphi_3 = \bigwedge_{\mathbf{p} \in \{+,-\}} \forall \pi \in X_d$ .  $\exists \pi' \in X_d$ .  $\mathbf{p}_{\pi} \to (\mathbf{p}_{\pi'} \land \mathbf{F}(\mathbf{x}_{\pi} \land \mathbf{X} \mathbf{x}_{\pi'}))$ : for both  $\mathbf{p} \in \{+,-\}$ , if the type  $\mathbf{p}$  trace  $\{\mathbf{p}\}^n \{\mathbf{x}, \mathbf{p}\} \{\mathbf{p}\}^{\omega}$  is in a model for some  $n \in \mathbb{N}$ , then also  $\{\mathbf{p}\}^{n+1} \{\mathbf{x}, \mathbf{p}\} \{\mathbf{p}\}^{\omega}$ .

The formulas  $\varphi_1, \varphi_2, \varphi_3$  are similar to the formulas  $\psi_1, \psi_2, \psi_3$  from Example 1. So, every model of the first four conjuncts contains  $\{\{+\}^n \{\mathbf{x}, +\} \{+\}^\omega \mid n \in \mathbb{N}\}$  and  $\{\{-\}^n \{\mathbf{x}, -\} \{-\}^\omega \mid n \in \mathbb{N}\}$  as subsets, and no other type + or type - traces.

Now, consider a set T of traces over AP (recall that second-order quantification ranges over arbitrary sets, not only over subsets of the universe of discourse). We say that T is contradiction-free if there is no  $n \in \mathbb{N}$  such that  $\{+\}^n \{\mathbf{x}, +\} \{+\}^\omega \in T$  and  $\{-\}^n \{\mathbf{x}, -\} \{-\}^\omega \in T$ . Furthermore, a trace t over AP is consistent with a contradiction-free T if

- (C1)  $\{+\}^n \{\mathbf{x},+\} \{+\}^\omega \in T \text{ implies } \mathbf{x} \in t(n) \text{ and }$
- (C2)  $\{-\}^n \{\mathbf{x}, -\} \{-\}^\omega \in T \text{ implies } \mathbf{x} \notin t(n).$

Note that T does not necessarily specify the truth value of  $\mathbf{x}$  in every position of t, i.e., in those positions  $n \in \mathbb{N}$  where neither  $\{+\}^n \{\mathbf{x},+\} \{+\}^\omega$  nor  $\{-\}^n \{\mathbf{x},-\} \{-\}^\omega$  are in T. Nevertheless, for every trace t over  $\{\mathbf{x}\}$  there is a contradiction-free T such that the  $\{\mathbf{x}\}$ -projection of every trace t' over AP that is consistent with T is equal to t.

• Hence, we define  $\varphi_4$  as the formula

$$\forall X. \quad \overbrace{[\forall \pi \in X. \forall \pi' \in X. (+_{\pi} \land \neg_{\pi'}) \to \neg \mathbf{F}(\mathbf{x}_{\pi} \land \mathbf{x}_{\pi'})]}^{X \text{ is contradiction-free}} \to \exists \pi'' \in X. \forall \pi'' \in X. \mathbf{s}_{\pi''} \land \underbrace{(+_{\pi'''} \to \mathbf{F}(\mathbf{x}_{\pi'''} \land \mathbf{x}_{\pi''}))}_{(C1)} \land \underbrace{(\neg_{\pi'''} \to \mathbf{F}(\mathbf{x}_{\pi'''} \land \neg \mathbf{x}_{\pi''}))}_{(C2)},$$

expressing that for every contradiction-free set of traces T, there is a type **s** trace t'' in the model (note that  $\pi''$  is required to be in  $X_d$ ) that is consistent with T.

While  $\varphi_{allSets}$  is not in prenex normal form, it can easily be turned into an equivalent formula in prenex normal form (at the cost of readability).

Now, the set

$$\begin{split} T_{allSets} &= \{\{+\}^n \{\mathbf{x}, +\}\{+\}^{\omega} \mid n \in \mathbb{N}\} \cup \{\{-\}^n \{\mathbf{x}, -\}\{-\}^{\omega} \mid n \in \mathbb{N}\} \cup \\ &\{(t(0) \cup \{\mathbf{s}\})(t(1) \cup \{\mathbf{s}\})(t(2) \cup \{\mathbf{s}\}) \cdots \mid t \in (2^{\{\mathbf{x}\}})^{\omega}\} \end{split}$$

of traces satisfies  $\varphi_{allSets}$ . On the other hand, every model of  $\varphi_{allSets}$  must indeed contain  $T_{allSets}$  as a subset, as  $\varphi_{allSets}$  requires the existence of all of its traces in the model. Finally, due to  $\varphi_0$  and  $\varphi_1$ , a model cannot contain any traces that are not in  $T_{allSets}$ , i.e.,  $T_{allSets}$  is the unique model of  $\varphi_{allSets}$ .

To conclude, we just remark that

$$\{(t(0) \cup \{\mathbf{s}\})(t(1) \cup \{\mathbf{s}\})(t(2) \cup \{\mathbf{s}\}) \cdots \mid t \in (2^{\{\mathbf{x}\}})^{\omega}\} \subseteq T_{allSets}$$

has indeed cardinality  $\mathfrak{c}$ , as  $(2^{\{x\}})^{\omega}$  has cardinality  $\mathfrak{c}$ .

Finally, let us consider closed-world semantics. We can restrict the second-order quantifier in  $\varphi_4$  (the only one in  $\varphi_{allSets}$ ) to subsets of the universe of discourse, as the set  $T = \{\{+\}^n \{\mathbf{x}, +\} \{+\}^\omega \mid n \in \mathbb{N}\} \cup \{\{-\}^n \{\mathbf{x}, -\} \{-\}^\omega \mid n \in \mathbb{N}\}\}$  of traces (which is a subset of every model) is already *rich* enough to encode every subset of  $\mathbb{N}$  by an appropriate contradiction-free subset of T. Thus,  $\varphi_{allSets}$  has the unique model  $T_{allSets}$  even under closed-world semantics.

#### C Proof of Theorem 2 and Corollary 1

Recall that we need to show that the Hyper<sup>2</sup>LTL satisfiability problem is polynomial-time equivalent to truth in third-order arithmetic and that the lower bound holds even for  $X_a$ -free sentences under standard semantics and for closed-world semantics.

We rely on the implementation of addition and multiplication in HyperLTL following Fortin et al. [12]. Let  $AP_{arith} = \{arg1, arg2, res, add, mult\}$  and let  $T_{(+,\cdot)}$  be the set of all traces  $t \in (2^{AP_{arith}})^{\omega}$  such that

- there are unique  $n_1, n_2, n_3 \in \mathbb{N}$  with  $\arg 1 \in t(n_1)$ ,  $\arg 2 \in t(n_2)$ , and  $\operatorname{res} \in t(n_3)$ , and
- either add  $\in t(n)$ , mult  $\notin t(n)$  for all n, and  $n_1 + n_2 = n_3$ , or mult  $\in t(n)$ , add  $\notin t(n)$  for all n, and  $n_1 \cdot n_2 = n_3$ .

**Proposition 3** (Theorem 5.5 of [12]). There is a satisfiable HyperLTL sentence  $\varphi_{(+,\cdot)}$  such that the AP<sub>arith</sub>-projection of every model of  $\varphi_{(+,\cdot)}$  is  $T_{(+,\cdot)}$ .

Proof of Theorem 2. We begin with the lower bound by reducing truth in third-order arithmetic to Hyper<sup>2</sup>LTL satisfiability: we present a polynomial-time translation from sentences  $\varphi$  of third-order arithmetic to Hyper<sup>2</sup>LTL sentences  $\varphi'$  such that  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi$  if and only if  $\varphi'$  is satisfiable.

Given a third-order sentence  $\varphi$ , we define

$$\varphi' = \exists X_{allSets}. \ \exists X_{arith}. \ (\varphi_{allSets}[X_d/X_{allSets}] \land \varphi'_{(+,\cdot)} \land hyp(\varphi))$$

where

- $\varphi_{allSets}[X_d/X_{allSets}]$  is the Hyper<sup>2</sup>LTL sentence from the proof of Theorem 1 where every occurrence of  $X_d$  is replaced by  $X_{allSets}$  and thus enforces every subset of  $\mathbb{N}$  to be encoded in the interpretation of  $X_{allSets}$  (as introduced in the proof of Theorem 1),
- $\varphi'_{(+,\cdot)}$  is the Hyper<sup>2</sup>LTL formula obtained from the HyperLTL formula  $\varphi_{(+,\cdot)}$  by replacing each quantifier  $\exists \pi \ (\forall \pi, \text{ respectively})$  by  $\exists \pi \in X_{arith} \ (\forall \pi \in X_{arith}, \text{ respectively})$  and thus enforces that  $X_{arith}$  is interpreted by a set whose AP<sub>arith</sub>-projection is  $T_{(+,\cdot)}$ , and

where  $hyp(\varphi)$  is defined inductively as follows:

• For third-order variables  $\mathcal{Y}$ ,

$$hyp(\exists \mathcal{Y}. \ \psi) = \exists X_{\mathcal{Y}}. \ (\forall \pi \in X_{\mathcal{Y}}. \ \exists \pi' \in X_{allSets}. \ \pi =_{\{+,-,\mathbf{s},\mathbf{x}\}} \pi' \land \mathbf{s}_{\pi}) \land hyp(\psi).$$

• For third-order variables  $\mathcal{Y}$ ,

$$hyp(\forall \mathcal{Y}. \ \psi) = \forall X_{\mathcal{Y}}. \ (\forall \pi \in X_{\mathcal{Y}}. \ \exists \pi' \in X_{allSets}. \ \pi =_{\{+,-,\mathbf{s},\mathbf{x}\}} \pi' \land \mathbf{s}_{\pi}) \to hyp(\psi).$$

- For second-order variables Y,  $hyp(\exists Y, \psi) = \exists \pi_Y \in X_{allSets}$ .  $\mathbf{s}_{\pi_Y} \wedge hyp(\psi)$ .
- For second-order variables Y,  $hyp(\forall Y, \psi) = \forall \pi_Y \in X_{allSets}$ .  $\mathbf{s}_{\pi_Y} \to hyp(\psi)$ .
- For first-order variables y,

$$hyp(\exists y. \ \psi) = \exists \pi_y \in X_{allSets}. \ \mathbf{s}_{\pi_y} \land [(\neg \mathbf{x}_{\pi_y}) \mathbf{U}(\mathbf{x}_{\pi_y} \land \mathbf{X} \mathbf{G} \neg \mathbf{x}_{\pi_y})] \land hyp(\psi).$$

• For first-order variables y,

$$hyp(\forall y. \ \psi) = \forall \pi_y \in X_{allSets}. \ (\mathbf{s}_{\pi_y} \land [(\neg \mathbf{x}_{\pi_y}) \mathbf{U}(\mathbf{x}_{\pi_y} \land \mathbf{X} \mathbf{G} \neg \mathbf{x}_{\pi_y})]) \to hyp(\psi).$$

- $hyp(\psi_1 \lor \psi_2) = hyp(\psi_1) \lor hyp(\psi_2).$
- $hyp(\neg\psi) = \neg hyp(\psi).$
- For second-order variables Y and third-order variables  $\mathcal{Y}$ ,

$$hyp(Y \in \mathcal{Y}) = \exists \pi \in X_{\mathcal{Y}}. \ \mathbf{G}(\mathbf{x}_{\pi_Y} \leftrightarrow \mathbf{x}_{\pi}).$$

- For first-order variables y and second-order variables Y,  $hyp(y \in Y) = \mathbf{F}(\mathbf{x}_{\pi_u} \wedge \mathbf{x}_{\pi_Y})$ .
- For first-order variables  $y, y', hyp(y < y') = \mathbf{F}(\mathbf{x}_{\pi_y} \wedge \mathbf{X} \mathbf{F} \mathbf{x}_{\pi_{y'}}).$
- For first-order variables  $y_1, y_2, y$ ,

$$hyp(y_1 + y_2 = y) = \exists \pi \in X_{arith}. \ \texttt{add}_{\pi} \wedge \mathbf{F}(\texttt{arg1}_{\pi} \wedge \mathtt{x}_{\pi_{y_1}}) \wedge \mathbf{F}(\texttt{arg2}_{\pi} \wedge \mathtt{x}_{\pi_{y_2}}) \wedge \mathbf{F}(\texttt{res}_{\pi} \wedge \mathtt{x}_{\pi_{y_1}}).$$

• For first-order variables  $y_1, y_2, y_1$ ,

$$hyp(y_1 \cdot y_2 = y) = \exists \pi \in X_{arith}. \ \texttt{mult}_{\pi} \land \mathbf{F}(\texttt{arg1}_{\pi} \land \mathtt{x}_{\pi_{y_1}}) \land \mathbf{F}(\texttt{arg2}_{\pi} \land \mathtt{x}_{\pi_{y_2}}) \land \mathbf{F}(\texttt{res}_{\pi} \land \mathtt{x}_{\pi_{y_1}})$$

While  $\varphi'$  is not in prenex normal form, it can easily be brought into prenex normal form, as there are no quantifiers under the scope of a temporal operator.

As we are evaluating  $\varphi'$  w.r.t. standard semantics and the variable  $X_a$  (interpreted with the model) does not occur in  $\varphi'$ , satisfaction of  $\varphi'$  is independent of the model, i.e., for all sets T, T' of traces,  $T \models \varphi'$  if and only if  $T' \models \varphi'$ . So, let us fix some set T of traces. An induction shows that  $(\mathbb{N}, +, \cdot, <, \in)$  satisfies  $\varphi$  if and only if T satisfies  $\varphi'$ . Altogether we obtain the desired equivalence between  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi$  and  $\varphi'$  being satisfiable.

For the upper bound, we conversely reduce Hyper<sup>2</sup>LTL satisfiability to truth in third-order arithmetic: we present a polynomial-time translation from Hyper<sup>2</sup>LTL sentences  $\varphi$  to sentences  $\varphi'$  of third-order arithmetic such that  $\varphi$  is satisfiable if and only if  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi'$ . Here, we assume AP to be fixed, so that we can use |AP| as a constant in our formulas (which is definable in arithmetic).

Let  $pair: \mathbb{N} \times \mathbb{N} \to \mathbb{N}$  denote Cantor's pairing function defined as  $pair(i, j) = \frac{1}{2}(i + j)(i + j + 1) + j$ , which is a bijection. Furthermore, fix some bijection  $e: AP \to \{0, 1, \dots, |AP| - 1\}$ . Then, we encode a trace  $t \in (2^{AP})^{\omega}$  by the set  $S_t = \{pair(j, e(\mathbf{p})) \mid j \in \mathbb{N} \text{ and } \mathbf{p} \in t(j)\} \subseteq \mathbb{N}$ . As *pair* is a bijection, we have that  $t \neq t'$  implies  $S_t \neq S_{t'}$ . While not every subset of  $\mathbb{N}$  encodes some trace t, the first-order formula

$$\varphi_{isTrace}(Y) = \forall x. \ \forall y. \ y \ge |AP| \to pair(x, y) \notin Y$$

checks if a set does encode a trace. Here, we use *pair* as syntactic sugar, which is possible as the definition of *pair* only uses addition and multiplication.

As (certain) sets of natural numbers encode traces, sets of (certain) sets of natural numbers encode sets of traces. This is sufficient to reduce Hyper<sup>2</sup>LTL to third-order arithmetic, which allows the quantification over sets of sets of natural numbers. Before we present the translation, we need to introduce some more auxiliary formulas:

• Let  $\mathcal{Y}$  be a third-order variable (i.e.,  $\mathcal{Y}$  ranges over sets of sets of natural numbers). Then, the formula

$$\varphi_{onlyTraces}(\mathcal{Y}) = \forall Y. \ Y \in \mathcal{Y} \to \varphi_{isTrace}(Y)$$

checks if a set of sets of natural numbers only contains sets encoding a trace.

• Further, the formula

$$\varphi_{allTraces}(\mathcal{Y}) = \varphi_{onlyTraces}(\mathcal{Y}) \land \forall Y. \ \pi_{isTrace}(Y) \to Y \in \mathcal{Y}$$

checks if a set of sets of natural numbers contains exactly the sets encoding a trace.

Now, we are ready to define our encoding of Hyper<sup>2</sup>LTL in third-order arithmetic. Given a Hyper<sup>2</sup>LTL sentence  $\varphi$ , let

$$\varphi' = \exists \mathcal{Y}_a. \ \exists \mathcal{Y}_d. \ \varphi_{allTraces}(\mathcal{Y}_a) \land \varphi_{onlyTraces}(\mathcal{Y}_d) \land (ar(\varphi))(0)$$

where  $ar(\varphi)$  is defined inductively as presented below. Note that  $\varphi'$  requires  $\mathcal{Y}_a$  to contain exactly the encodings of all traces (i.e., it corresponds to the distinguished Hyper<sup>2</sup>LTL variable  $X_a$  in the following translation) and  $\mathcal{Y}_d$  is an existentially quantified set of trace encodings (i.e., it corresponds to the distinguished Hyper<sup>2</sup>LTL variable  $X_d$  in the following translation).

In the inductive definition of  $ar(\varphi)$ , we will employ a free first-order variable *i* to denote the position at which the formula is to be evaluated to capture the semantics of the temporal operators. As seen above, in  $\varphi'$ , this free variable is set to zero in correspondence with the Hyper<sup>2</sup>LTL semantics.

- $ar(\exists X. \psi) = \exists \mathcal{Y}_X. \varphi_{onlyTraces}(\mathcal{Y}_X) \wedge ar(\psi)$ . Here, the free variable of  $ar(\exists X. \psi)$  is the free variable of  $ar(\psi)$ .
- $ar(\forall X. \psi) = \forall \mathcal{Y}_X. \varphi_{onlyTraces}(\mathcal{Y}_X) \to ar(\psi)$ . Here, the free variable of  $ar(\forall X. \psi)$  is the free variable of  $ar(\psi)$ .
- $ar(\exists \pi \in X, \psi) = \exists Y_{\pi}, Y_{\pi} \in \mathcal{Y}_X \land ar(\psi)$ . Here, the free variable of  $ar(\exists \pi \in X, \psi)$  is the free variable of  $ar(\psi)$ .
- $ar(\forall \pi \in X, \psi) = \forall Y_{\pi}, Y_{\pi} \in \mathcal{Y}_X \to ar(\psi)$ . Here, the free variable of  $ar(\forall \pi \in X, \psi)$  is the free variable of  $ar(\psi)$ .
- $ar(\psi_1 \vee \psi_2) = ar(\psi_1) \vee ar(\psi_2)$ . Here, we require that the free variables of  $ar(\psi_1)$  and  $ar(\psi_2)$  are the same (which can always be achieved by variable renaming), which is then also the free variable of  $ar(\psi_1 \vee \psi_2)$ .
- $ar(\neg \psi) = \neg ar(\psi)$ . Here, the free variable of  $ar(\neg \psi)$  is the free variable of  $\neg ar(\psi)$ .
- $ar(\mathbf{X}\psi) = (i' = i+1) \wedge ar(\psi)$ , where i' is the free variable of  $ar(\psi)$  and i is the free variable of  $ar(\mathbf{X}\psi)$ .
- $ar(\psi_1 \mathbf{U} \psi) = \exists i_1 . i_1 \geq i \land ar(\psi_1) \land \forall i_2 . (i \leq i_2 \land i_2 < i_1) \rightarrow ar(\psi_2)$ , where  $i_1$  is the free variable of  $ar(\psi_1), i_2$  is the free variable of  $ar(\psi_2)$ , and i is the free variable of  $ar(\psi_1 \mathbf{U} \psi_2)$ .

•  $ar(\mathbf{p}_{\pi}) = pair(i, e(\mathbf{p})) \in Y_{\pi}$ , where  $e: AP \to \{0, 1, \dots, |AP| - 1\}$  is the encoding of propositions by natural numbers introduced above. Note that *i* is the free variable of  $ar(a_{\pi})$ .

Now, an induction shows that  $\Pi_{\emptyset}[X_a \to (2^{AP})^{\omega}, X_d \mapsto T] \models \varphi$  if and only if  $(\mathbb{N}, +, \cdot, <, \in)$  satisfies  $ar(\varphi)$  when the variable  $\mathcal{Y}_a$  is interpreted by the encoding of  $(2^{AP})^{\omega}$  and  $\mathcal{Y}_d$  is interpreted by the encoding of T. Hence,  $\varphi$  is indeed satisfiable if and only if  $(\mathbb{N}, +, \cdot, <, \in)$  satisfies  $\varphi'$ .

Recall that we have, in the lower bound proof above, turned a sentence  $\varphi$  of third-order arithmetic into a Hyper<sup>2</sup>LTL sentence  $\varphi'$  such that  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi$  if and only if  $\varphi'$  is satisfiable. In fact, we have constructed  $\varphi'$  such that if it is satisfiable, then every set of traces satisfies.

Under closed-world semantics the second-order quantifiers in  $\varphi'$  range over subsets of the model. Hence, if  $T = (2^{AP})^{\omega}$ , then we have  $T \models \varphi'$  if and only if  $\varphi'$  is satisfiable. Thus, the lower bound holds even under closed-world semantics. Together with Lemma 1 we obtain Corollary 1.

## D Proof of Theorem 3 and Corollary 2

Recall that we need to show that the Hyper<sup>2</sup>LTL finite-state satisfiability problem is polynomial-time equivalent to truth in third-order arithmetic and that the lower bound holds even for  $X_a$ -free sentences under standard semantics and for closed-world semantics.

Proof of Theorem 3. For the lower bound under standard semantics, we reduce truth in third-order arithmetic to Hyper<sup>2</sup>LTL finite-state satisfiability: we present a polynomial-time translation from sentences  $\varphi$  of third-order arithmetic to Hyper<sup>2</sup>LTL sentences  $\varphi'$  such that  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi$  if and only if  $\varphi'$  is satisfied by a finite transition system.

So, let  $\varphi$  be a sentence of third-order arithmetic. Recall that in the proof of Theorem 2, we have shown how to construct from  $\varphi$  the Hyper<sup>2</sup>LTL sentence  $\varphi'$  such that the following three statements are equivalent:

- $(\mathbb{N}, +, \cdot, <, \in) \models \varphi$ .
- $\varphi'$  is satisfiable.
- $\varphi'$  is satisfied all sets T of traces (and in particular by some finite-state transition system).

Thus, the lower bound follows from Theorem 2.

For the upper bound, we conversely reduce Hyper<sup>2</sup>LTL finite-state satisfiability to truth in third-order arithmetic: we present a polynomial-time translation from Hyper<sup>2</sup>LTL sentences  $\varphi$  to sentences  $\varphi''$  of third-order arithmetic such that  $\varphi$  is satisfied by a finite transition system if and only if  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi''$ .

Recall that in the proof of Theorem 2, we have constructed a Hyper<sup>2</sup>LTL sentence

$$\varphi' = \exists \mathcal{Y}_a. \ \exists \mathcal{Y}_d. \ \varphi_{allTraces}(\mathcal{Y}_a) \land \varphi_{onlyTraces}(\mathcal{Y}_d) \land (ar(\varphi))(0)$$

where  $\mathcal{Y}_a$  represents the distinguished Hyper<sup>2</sup>LTL variable  $X_a$ ,  $\mathcal{Y}_d$  represents the distinguished Hyper<sup>2</sup>LTL variable  $X_d$ , and where  $ar(\varphi)$  is the encoding of  $\varphi$  in Hyper<sup>2</sup>LTL.

To encode the general satisfiability problem it was sufficient to express that  $\mathcal{Y}_d$  only contains traces. Here, we now require that  $\mathcal{Y}_d$  contains exactly the traces of some finite transition system, which can easily be expressed in second-order arithmetic<sup>3</sup> as follows.

We begin with a formula  $\varphi_{isTS}(n, E, I, \ell)$  expressing that the second-order variables E, I, and  $\ell$  encode a transition system with set  $\{0, 1, \ldots, n-1\}$  of vertices. Our encoding will make extensive use of the pairing function introduced in the proof of Theorem 2. Formally, we define  $\varphi_{isTS}(n, E, I, \ell)$  as the conjunction of the following formulas (where all quantifiers are first-order and we use *pair* as syntactic sugar):

•  $\forall y. \ y \in E \to \exists v. \ \exists v'. \ (v < n \land v' < n \land y = pair(v, v'))$ : edges are pairs of vertices.

 $<sup>^{3}</sup>$ With a little more effort, and a little less readability, first-order suffices for this task, as finite transition systems can be encoded by natural numbers.

- $\forall v. v < n \rightarrow \exists v'. (v' < n \land pair(v, v') \in E)$ : every vertex has a successor.
- $\forall v. v \in I \rightarrow v < n$ : the set of initial vertices is a subset of the set of all vertices.
- $\forall y. \ y \in \ell \to \exists v. \exists p. \ (v < n \land p < |AP| \land y = pair(v, p))$ : the labeling of v by p is encoded by the pair (v, p). Here, we again assume AP to be fixed and therefore can use |AP| as a constant.

Next, we define  $\varphi_{isPath}(P, n, E, I)$ , expressing that the second-order variable P encodes a path through the transition system encoded by n, E, and I, as the conjunction of the following formulas:

- $\forall j. \exists v. (v < n \land pair(j, v) \in P \land \neg \exists v'. (v' \neq v \land pair(j, v') \in P))$ : the fact that at position j the path visits vertex v is encoded by the pair (j, v). Exactly one vertex is visited at each position.
- $\exists v. v \in I \land pair(0, v) \in P$ : the path starts in an initial vertex.
- $\forall j. \exists v. \exists v'. pair(j, v) \in P \land pair(j + 1, v') \in P \land pair(v, v') \in E$ : successive vertices in the path are indeed connected by an edge.

Finally, we define  $\varphi_{traceOf}(T, P, \ell)$ , expressing that the second-order variable T encodes the trace (using the encoding from the proof of Theorem 2) of the path encoded by the second-order variable P, as the following formula:

•  $\forall j. \forall p. pair(j,p) \in T \leftrightarrow (\exists v. (j,v) \in P \land (v,p) \in \ell)$ : a proposition holds in the trace at position j if and only if it is in the labeling of the j-th vertex of the path.

Now, we define the sentence  $\varphi''$  as

$$\exists \mathcal{Y}_{d}. \exists \mathcal{Y}_{d}. \varphi_{allTraces}(\mathcal{Y}_{d}) \land \varphi_{onlyTraces}(\mathcal{Y}_{d}) \land \\ \underbrace{\exists n. \exists E. \exists I. \exists \ell. \varphi_{isTS}(n, E, I, \ell) \land \\ \text{there exists a transition system } \mathfrak{T} \\ \underbrace{(\forall T. T \in \mathcal{Y}_{d} \rightarrow \exists P. (\varphi_{isPath}(P, n, E, I) \land \varphi_{traceOf}(T, P, \ell)))}_{\mathcal{Y}_{d} \text{ contains only traces of paths through } \mathfrak{T} \\ \underbrace{(\forall P. (\varphi_{isPath}(P, n, E, I) \rightarrow \exists T. T \in \mathcal{Y}_{d} \land \varphi_{traceOf}(T, P, \ell)))}_{\mathcal{Y}_{d} \text{ contains all traces of paths through } \mathfrak{T}. \\ (ar(\varphi))(0), \end{aligned}$$

which holds in  $(\mathbb{N}, +, \cdot, <, \in)$  if and only if  $\varphi$  is satisfied by a finite transition system.

As for the general case, the sentence  $\varphi'$  we have constructed above is satisfiable under closed-world semantics if and only if  $(2^{AP})^{\omega}$  satisfies it under closed-world semantics, which is the language of a finite transition system. With Lemma 1, we then obtain Corollary 2.

Let us also just remark that the proof of Theorem 3 can easily be adapted to show that other natural variations of the satisfiability problem are also polynomial-time equivalent to truth in third-order arithmetic, e.g., satisfiability by countable transition systems, satisfiability by finitely branching transition systems, etc. In fact, as long as a class C of transition systems is definable in third-order arithmetic, the Hyper<sup>2</sup>LTL satisfiability problem restricted to transition systems in C is reducible to truth in third-order arithmetic. Similarly, truth in third-order arithmetic is reducible to Hyper<sup>2</sup>LTL satisfiability for every nonempty class of models (w.r.t. standard semantics) and to every class of models containing at least one whose language contains  $T_{allSets} \cup T_{arith}$  (w.r.t. closed-world semantics).

#### E Proof of Theorem 4 and Corollary 3

Recall that we need to prove that the Hyper<sup>2</sup>LTL model-checking problem is polynomial-time equivalent to truth in third-order arithmetic and that the lower bound already holds for  $X_a$ -free sentences under standard semantics and for closed-world semantics.

Proof of Theorem 4. For the lower bound, we reduce truth in third-order arithmetic to the Hyper<sup>2</sup>LTL model-checking problem: we present a polynomial-time translation from sentences  $\varphi$  of third-order arithmetic to pairs  $(\mathfrak{T}, \varphi')$  of a finite transition system  $\mathfrak{T}$  and a Hyper<sup>2</sup>LTL sentence  $\varphi'$  such that  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi$  if and only if  $\mathfrak{T} \models \varphi'$ .

In the proof of Theorem 2 we have, given a sentence  $\varphi$  of third-order arithmetic, constructed a Hyper<sup>2</sup>LTL sentence  $\varphi'$  such that  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi$  if and only if every set T of traces satisfies  $\varphi'$  (i.e., satisfaction is independent of the model). Thus, we obtain the lower bound by mapping  $\varphi$  to  $\varphi'$  and  $\mathfrak{T}^*$ , where  $\mathfrak{T}^*$  is some fixed transition system.

For the upper bound, we reduce the Hyper<sup>2</sup>LTL model-checking problem to truth in third-order arithmetic: we present a polynomial-time translation from pairs  $(\mathfrak{T}, \varphi)$  of a finite transition system and a Hyper<sup>2</sup>LTL sentence  $\varphi$  to sentences  $\varphi'$  of third-order arithmetic such that  $\mathfrak{T} \models \varphi$  if and only if  $(\mathbb{N}, +, \cdot, <, \in) \models \varphi'$ .

In the proof of Theorem 3, we have constructed, from a Hyper<sup>2</sup>LTL sentence  $\varphi$ , a sentence  $\varphi'$  of thirdorder arithmetic that expresses the existence of a finite transition system that satisfies  $\varphi$ . We obtain the desired upper bound by modifying  $\varphi'$  to replace the existential quantification of the transition system by hardcoding  $\mathfrak{T}$  instead.

Again, the results for closed-world semantics follow as in the case of finite-state satisfiability: For the lowe bound, we just have to pick  $\mathfrak{T}^*$  such that its set of traces contains  $T_{allSets} \cup T_{arith}$ .

#### F Proof of Theorem 5

Recall that we need to show that there is a satisfiable  $X_a$ -free Hyper<sup>2</sup>LTL<sub>fp</sub> sentence that only has models of cardinality  $\mathfrak{c}$ , under standard and closed-world semantics.

*Proof.* We adapt the proof of Theorem 1 to  $\text{Hyper}^2 \text{LTL}_{fp}$ . Recall that we have constructed the formula  $\varphi_{allSets} = \varphi_0 \land \cdots \land \varphi_4$  whose unique model is uncountable. The subformulas  $\varphi_0, \ldots, \varphi_3$  of  $\varphi_{allSets}$  are first-order, so let us consider  $\varphi_4$ . Recall that  $\varphi_4$  has the form

$$\forall X. \ [\forall \pi \in X. \ \forall \pi' \in X. \ (+_{\pi} \land -_{\pi'}) \to \neg \mathbf{F}(\mathbf{x}_{\pi} \land \mathbf{x}_{\pi'})] \to \\ \exists \pi'' \in X_d. \ \forall \pi''' \in X. \ \mathbf{s}_{\pi''} \land (+_{\pi'''} \to \mathbf{F}(\mathbf{x}_{\pi'''} \land \mathbf{x}_{\pi''})) \land (-_{\pi'''} \to \mathbf{F}(\mathbf{x}_{\pi'''} \land \neg \mathbf{x}_{\pi''})),$$

expressing that for every contradiction-free set of traces T, there is a type **s** trace t'' in the model that is consistent with T. Here, X ranges over arbitrary sets T of traces. However, this is not necessary. Consider the formula

$$\varphi'_{4} = \forall (X, \lambda, \varphi_{conFree}). \exists \pi'' \in X_{d}. \forall \pi''' \in X.$$
$$\mathbf{s}_{\pi''} \wedge (\mathbf{+}_{\pi'''} \to \mathbf{F}(\mathbf{x}_{\pi'''} \wedge \mathbf{x}_{\pi''})) \wedge (\mathbf{-}_{\pi'''} \to \mathbf{F}(\mathbf{x}_{\pi'''} \wedge \neg \mathbf{x}_{\pi''})),$$

with

$$\varphi_{conFree} = \forall \pi \in X. \ \forall \pi' \in X. \ (+_{\pi} \land -_{\pi'}) \to \neg \mathbf{F}(\mathbf{x}_{\pi} \land \mathbf{x}_{\pi'})$$

expressing that X is contradiction-free. In  $\varphi'_4$  the set variable X only ranges over maximal contradiction-free sets of traces, i.e., those that contain for each n either  $\{+\}^n \{\mathbf{x}, +\} \{+\}^\omega$  or  $\{-\}^n \{\mathbf{x}, -\} \{-\}^\omega$ .

But even with the restriction to such maximal sets,  $\varphi'_4$  still requires that a model of  $\varphi'_{allSets} = \varphi_0 \wedge \cdots \varphi_3 \wedge \varphi'_4$  contains the encoding of every subset of  $\mathbb{N}$  by a type **s** trace, as every subset of  $\mathbb{N}$  is captured by a maximal contradiction-free set of traces.

As in the proof of Theorem 1, this construction is correct for standard and closed-world semantics, as the other subformulas already ensure that the models have enough traces to enforce all subsets of natural numbers to be in the model.  $\hfill \Box$ 

#### G Proof of Theorem 6 and Corollary 4

Recall that we need to show that  $\text{Hyper}^2 \text{LTL}_{fp}$  satisfiability, finite-state satisfiability, and model-checking are polynomial-time equivalent to truth in third-order arithmetic and that the lower bound holds even for  $X_a$ -free sentences and closed-world semantics.

*Proof of Theorem 6.* The upper bounds follow directly from the analogous upper bounds for Hyper<sup>2</sup>LTL and Proposition 2.

For the lower bounds, let us fix some set AP' not containing the propositions  $+, -, \mathbf{s}, \mathbf{x}$  used to construct  $\varphi'_{allSets}$  and let AP = AP'  $\cup \{+, -, \mathbf{s}, \mathbf{x}\}$ . Then, due to Theorem 5, we have

 $\{T \mid T \text{ is the AP'-projection of some } T \in \text{sol}(\Pi, (X, \Upsilon, \varphi'_{allSets}))\}$ 

is equal to  $2^{(2^{AP'})^{\omega}}$ , as there is a bijection between  $(2^{AP})^{\omega}$  and  $(2^{AP'})^{\omega}$  and we are restricting the quantifiers to largest sets satisfying  $\varphi'_{allSets}$ .

Hence, we can use guarded quantification to simulate general quantification. This allows us to easily transfer all lower bounds for Hyper<sup>2</sup>LTL to Hyper<sup>2</sup>LTL<sub>fp</sub>: The lower bounds are obtained by adapting the reductions presented in the proofs of Theorem 2, Theorem 3, and Theorem 4 by replacing

- each existential second-order quantifier  $\exists X$  by  $\exists (X, \curlyvee, \varphi'_{allSets})$  and
- each universal second-order quantifier  $\forall X$  by  $\forall (X, \Upsilon, \varphi'_{allSets})$ .

Here, we just have to assume that the propositions in  $\varphi'_{allSets}$  do not appear in the formulas we are modifying, which can always be achieved by renaming propositions, if necessary. As explained above, the modified sentences with restricted quantification are equivalent to the original Hyper<sup>2</sup>LTL sentences constructed in the proofs of Theorem 2, Theorem 3, and Theorem 4, which implies the desired lower bounds.

Furthermore, the construction are correct both for standard and closed-world semantics, just as the constructions we modify here do.  $\hfill \Box$ 

## H Proof of Lemma 2

Recall that we need to show that every satisfiable  $X_{a}$ -free lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> sentence has a countable model.

*Proof.* Let

$$= \gamma_1 Q_1(Y_1, \Upsilon, \varphi_1^{\text{con}}), \ \gamma_2 Q_2(Y_2, \Upsilon, \varphi_2^{\text{con}}), \ \dots, \gamma_k Q_2(Y_k, \Upsilon, \varphi_k^{\text{con}}), \ \gamma_{k+1} \psi$$

be a satisfiable  $lfp-Hyper^2LTL_{fp}$  sentence, where

$$\varphi_j^{\text{con}} = \dot{\pi}_1 \triangleright Y_j \land \dots \land \dot{\pi}_n \triangleright Y_j \land \forall \ddot{\pi}_1 \in Z_1. \dots \forall \ddot{\pi}_{n'} \in Z_{n'}. \ \psi_j^{\text{step}} \to \ddot{\pi}_m \triangleright Y_j$$

We assume w.l.o.g. that each trace variable is quantified at most once in  $\varphi$ , which can always be achieved by renaming variables. This implies that for each trace variable  $\pi$  quantified in some  $\gamma_j$  or in some  $\varphi_j^{\text{con}}$ , there is a unique second-order variable  $X_{\pi}$  such that  $\pi$  ranges over  $X_{\pi}$ .

As  $\varphi$  is satisfiable, there exists a set T of traces such that  $T \models \varphi$ . We show that there is a countable  $R \subseteq T$  with  $R \models \varphi$ . Intuitively, we show that the smallest set that is closed under Skolem functions and the functions  $f_{\prod, j}$  (for certain assignments  $\Pi$ ) inducing the least fixed points has the desired properties.

So, let E be the set of existentially quantified trace variables in the  $\gamma_j$  and let, for each  $\pi \in E$ ,  $k_{\pi}$  denote the number of trace variables that are universally quantified before  $\pi$  (in any block  $\gamma_j$ ). As T satisfies  $\varphi$ , there is a Skolem function  $f_{\pi}: T^{k_{\pi}} \to T$  for each  $\pi \in E$ , i.e., functions witnessing  $T \models \varphi$  in the following sense:  $\Pi \models \psi$  for every  $\Pi$  where

- for each universally quantified trace variable  $\pi$  that appears in a  $\gamma_i$  we have  $\Pi(\pi) \in \Pi(X_{\pi})$ ,
- for each existentially quantified trace variable  $\pi$  that appears in a  $\gamma_j$ , we have  $\Pi(\pi) = f_{\pi}(\Pi(\pi_1), \ldots, \Pi(\pi_{k_{\pi}})) \in \Pi(X_{\pi})$ , where  $\pi_1, \ldots, \pi_{k_{\pi}}$  are the universally quantified trace variables that appear in some  $\gamma_j$  before  $\pi$ ,
- each second-order variable  $Y_j$  is mapped to  $lfp(\Pi, j)$ , and
- $X_d$  is mapped to T.

We fix such Skolem functions for the rest of the proof.

Given a set  $T' \subseteq T$ , we define

$$f_{\pi}(T') = \{ f_{\pi}(t_1, \dots, t_{k_{\pi}}) \mid t_1, \dots, t_{k_{\pi}} \in T' \}.$$

Also, we say that a variable assignment  $\Pi$  is a T'-assignment if

- $\Pi(X_d) = T',$
- $\Pi(Y_j) \subseteq T'$  for all  $Y_j$ ,
- $\Pi(\pi) \in T'$  for all trace variables  $\pi$  that are universally quantified in  $\varphi$ ,
- $\Pi(\pi) = f_{\pi}(\Pi(\pi_1), \dots, \Pi(\pi_{k_{\pi}}))$  for all trace variables  $\pi$  that are existentially quantified in  $\varphi$  (but no requirement on  $\Pi(\pi)$  being in T'!), and
- $\Pi$  is undefined for all variables that do not occur in  $\varphi$ .

Note that if T' is finite, then there are only finitely many T'-assignments. Now, we define  $R_0 = \emptyset$  and

$$R_{\ell+1} = R_{\ell} \cup \bigcup_{\pi} f_{\pi}(R_{\ell}) \cup \bigcup_{\Pi} \bigcup_{j=1}^{k} f_{\Pi,j}(R_{\ell})$$

where  $\pi$  in the first union ranges over all existentially quantified variables in the  $\gamma_j$  and  $\Pi$  in the second union ranges over all  $R_{\ell}$ -assignments. We claim that  $R = \bigcup_{\ell \in \mathbb{N}} R_{\ell}$  is countable and a model of  $\varphi$ . The first claim is straightforward, as an induction shows that each  $R_{\ell}$  is finite, which implies that R as a countable union of finite sets is countable. This relies on the fact that there are only finitely many  $R_{\ell}$ -assignments. Thus, there will only be finitely many traces added to  $R_{\ell}$  to obtain  $R_{\ell+1}$  from  $R_{\ell}$ .

So, let us show  $R \models \varphi$ . Note that  $t_1, \ldots, t_{k_\pi} \in R$  implies  $f_\pi(t_1, \ldots, t_{k_\pi}) \in R$  (we mark this claim by  $(\dagger)$ ): The  $t_i$  are already all in  $R_\ell$  for some  $\ell$ , which implies  $f_\pi(t_1, \ldots, t_{k_\pi}) \in R_{\ell+1} \subseteq R$ .

Now, let  $\Pi$  be a variable assignment such that

- $X_d$  is mapped to R,
- each second-order variable  $Y_j$  is mapped to  $lfp(\Pi, j)$ ,
- each universally quantified trace variable  $\pi$  is mapped to a trace in  $\Pi(X_{\pi})$  (which by construction is in R), and
- each existentially quantified variable  $\pi$  is mapped to  $f_{\pi}(\Pi(\pi_1), \ldots, \Pi(\pi_{k_{\pi}}))$ , which is in R due to  $(\dagger)$ , where  $\pi_1, \ldots, \pi_{k_{\pi}}$  are again the universally quantified trace variables before  $\pi$ .

Then, we have  $\Pi \models \psi$  as all existentially quantified variables are picked according to the Skolem functions. However, a priori, it might be that, for some existentially quantified  $\pi$ ,  $f_{\pi}(\Pi(\pi_1), \ldots, \Pi(\pi_{k_{\pi}}))$  is not in  $\Pi(X_{\pi})$ , as the Skolem functions are picked w.r.t. the model T, but here we apply them for the model R. Below, we show that this cannot be the case. With this result, an induction over the quantifier prefix shows that  $\{X_d \mapsto R\} \models \varphi$  (i.e.,  $R \models \varphi$ ), where the induction start is  $\Pi \models \psi$ .

So, let  $\pi$  be existentially quantified and define  $t^* = f_{\pi}(\Pi(\pi_1), \ldots, \Pi(\pi_{k_{\pi}}))$  for notational convenience. If  $X_{\pi}$  is  $X_d$ , then the result follows due to (†), as  $\Pi(X_d) = R$ . The only other possibility is  $X_{\pi} = Y_j$  for some j, i.e.,  $X_{\pi}$  is one of the second-order variables in  $\varphi$ .

From the variable assignment  $\Pi$ , we construct the variable assignment  $\Pi'$  that maps

- $X_d$  to T (recall that T is the model we started with),
- each second-order variable  $Y_i$  to  $lfp(\Pi', j)$ ,
- each universally quantified trace variable  $\pi$  to  $\Pi(\pi)$ , and
- each existentially quantified variable  $\pi$  to  $\Pi(\pi) = f_{\pi}(\Pi(\pi_1), \ldots, \Pi(\pi_{k_{\pi}})).$

As the  $f_{\pi}$  are Skolem functions witnessing  $T \models \varphi$ , we conclude that

$$t^* = \Pi'(\pi) = \Pi(\pi) = f_{\pi}(\Pi(\pi_1), \dots, \Pi(\pi_{k_{\pi}})) \in \Pi'(Y_j) = \operatorname{lfp}(\Pi', j),$$

i.e.,  $t^*$  is in the fixed point computed w.r.t.  $\Pi'(X_d) = T$ .

Let  $\operatorname{lfp}(\Pi', j) = \bigcup_{\ell \in \mathbb{N}} S'_{\ell}$  with  $S'_0 = \emptyset$  and  $S'_{\ell+1} = f_{\Pi',j}(S'_{\ell})$ . As  $t^* \in \operatorname{lfp}(\Pi', j)$ , there is some minimal  $\ell^* \geq 0$  such that  $t^* \in S'_{\ell^*}$ . If  $\ell^* > 0$ , then  $t^* \in f_{\Pi',j}(S_{\ell-1}, j)$ . This means there are traces  $t_i$  for the universally quantified variables  $\ddot{\pi}_i$  in  $\psi_j^{\text{step}}$  such that  $t_i \in \Pi'(Z_i)$  if  $Z_i \neq Y_j$  and  $t_i \in S'_{\ell-1}$  if  $Z_i = Y_j$  such that the  $t_i$  witness  $t^* \in S'_{\ell^*}$  via  $\Pi'[\ddot{\pi}_1 \mapsto t_1, \ldots, \dot{\pi}_{n'} \mapsto t_{n'}] \models \psi_j^{\text{step}}$ . Those  $t_i$  that are in  $S'_{\ell^*-1}$  again have such witnesses, some of which may be in  $S'_{\ell^*-2}$ , provided  $\ell^* > 1$ . This process can be continued until we end up with witnesses in  $S'_1$ . Thus, these witnesses must be of the form  $\Pi'(\dot{\pi})$  for variables  $\dot{\pi}$  that are quantified outside of  $\varphi_i^{\operatorname{con}}$ , i.e., in some block  $\gamma_{j'}$  with  $j' \leq j$ .

Let  $\operatorname{lfp}(\Pi, j) = \bigcup_{\ell \in \mathbb{N}} S_{\ell}$  be the fixed point computed w.r.t.  $\Pi$ , i.e.,  $S_0 = \emptyset$  and  $S_{\ell+1} = f_{\Pi,j}(S_{\ell})$ . Recall that  $\Pi$  and  $\Pi'$  coincide for the variables  $\dot{\pi}$  (because they are quantified outside of  $\varphi_j^{\operatorname{con}}$ ) and that the traces  $\Pi'(\dot{\pi}) = \Pi(\dot{\pi})$  are in R by the choice of  $\Pi$ , and therefore in some finite state of the computation of R.

Hence, the  $\Pi(\dot{\pi})$  are also in  $S_1 = f_{\Pi,j}(\emptyset)$ . Now, an induction over  $\ell$  shows that also all the traces in some  $S'_{\ell}$  witnessing  $t^* \in S'_{\ell^*}$  are also in R (as R is closed under the application of  $f_{\Pi'',j}$  for suitable assignments  $\Pi''$ ) and therefore also in  $S_{\ell}$ . Then, we also conclude  $t^* \in S_{\ell^*} = \mathrm{lfp}(\Pi, j) = \Pi(Y_j)$ .

#### I Proof of Theorem 7

Recall that we need to show that  $lfp-Hyper^2LTL_{fp}$  satisfiability for  $X_a$ -free sentences is  $\Sigma_1^1$ -complete.

*Proof.* Throughout this proof, we fix an  $X_a$ -free lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> sentence

$$\varphi = \gamma_1. \ Q_1(Y_1, \Upsilon, \varphi_1^{\text{con}}). \ \gamma_2. \ Q_2(Y_2, \Upsilon, \varphi_2^{\text{con}}). \ \dots \gamma_k. \ Q_k(Y_k, \Upsilon, \varphi_k^{\text{con}}). \ \gamma_{k+1}\psi,$$

where  $\psi$  is quantifier-free, and let  $\Phi$  denote the set of quantifier-free subformulas of  $\varphi$  (including those in the guards). As before, we assume w.l.o.g. that each trace variable is quantified at most once in  $\varphi$ , i.e., for each trace variable  $\pi$  quantified in some  $\gamma_j$  or in some  $\varphi_j^{\text{con}}$ , there is a unique second-order variable  $X_{\pi}$  such that  $\pi$  ranges over  $X_{\pi}$ .

The  $\Sigma_1^1$  lower bound already holds for HyperLTL satisfiability [11], as HyperLTL is a fragment of  $X_a$ -free lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> (see Remark 1). Hence, we focus in the following on the upper bound, which is a generalization of the corresponding upper bound for HyperLTL [11].

Due to Lemma 2,  $\varphi$  is satisfiable if and only if it has a countable model T. Thus, not only is T countable, but the second-order quantifiers range over subsets of T, i.e., over countable sets. Finally, recall that the least fixed point assigned to  $Y_j$  depends on the variable assignment to trace variables in the blocks  $\gamma_1, \ldots, \gamma_j$ , but not on the second-order variables  $Y_{j'}$  with j' < j, as their values are also uniquely determined by the variables in the blocks  $\gamma_1, \ldots, \gamma_{j'}$ . Let  $\Pi$  be a variable assignment whose domain contains all the trace variables of  $\varphi$ , and therefore in particular all free variables of  $\psi$ . Then,  $\Pi \models \psi$  if and only if there is a function  $e \colon \Phi \times \mathbb{N} \to \{0, 1\}$  with  $e(\psi, 0) = 1$  satisfying the following consistency conditions:

- $e(a_{\pi}, j) = 1$  if and only if  $a \in \Pi(\pi)(j)$ .
- $e(\neg \psi_1, j) = 1$  if and only if  $e(\psi_1, j) = 0$ .
- $e(\psi_1 \lor \psi_2, j) = 1$  if and only if  $e(\psi_1, j) = 1$  or  $e(\psi_2, j) = 1$ .
- $e(\mathbf{X}\psi_1, j) = 1$  if and only if  $e(\psi_1, j+1) = 1$ .
- $e(\psi_1 \mathbf{U} \psi_2, j) = 1$  if and only if there is a  $j' \ge j$  such that  $e(\psi_2, j') = 1$  and  $e(\psi_2, j'') = 1$  for all j'' in the range  $j \le j'' < j'$ .

In fact, there is exactly one function e satisfying these consistency conditions, namely the function  $e_{\varphi,\Pi}$  defined as

$$e_{\varphi,\Pi}(\psi',j) = \begin{cases} 1 & \text{if } \Pi[j,\infty) \models \psi' \\ 0 & \text{otherwise.} \end{cases}$$

To prove that the lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> satisfiability problem for  $X_a$ -free sentences is in  $\Sigma_1^1$ , we express, for a given  $X_a$ -free lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> sentence  $\varphi$  (encoded as a natural number), the existence of a countable set T of traces and a witness that T is indeed a model of  $\varphi$ . As we work with second-order arithmetic we can quantify only over natural numbers (type 0 objects) and sets of natural numbers (type 1 objects). To simplify our notation, we note that there is a bijection between finite sequences over  $\mathbb{N}$  and  $\mathbb{N}$  itself and that one can encode functions mapping natural numbers to natural numbers as sets of natural numbers via their graphs. As both can be implemented in arithmetic, we will freely use vectors of natural numbers, functions mapping natural numbers to natural numbers, and combinations of both.

Furthermore, as we only have to work with countable sets of traces, we can use natural numbers to "name" the traces. Hence, the restriction of a variable assignment to trace variables can be encoded by a vector of trace names, listing (in some fixed order), the names of the traces assigned to the trace variables. Finally, the countable sets assigned to the  $Y_j$  depend on the variable assignment to the trace variables quantified before  $Y_j$ , but not on the sets assigned to the  $Y_{j'}$  with j' < j. Thus we do not have to consider second-order variables in variable assignments: in the following, when we speak of a variable assignment we only consider those that are undefined for all second-order variables. Let k' denote the number of trace variables in  $\varphi$ . Then, variable assignments are encoded by vectors in  $\mathbb{N}^{k'}$ .

Now, given  $\varphi$  we express the existence of the following type 1 objects:

- A countable set of traces over the propositions of  $\varphi$  encoded as a function T from  $\mathbb{N} \times \mathbb{N}$  to  $\mathbb{N}$ , mapping trace names (i.e., natural numbers) and positions to (encodings of) subsets of the set of propositions appearing in  $\varphi$ .
- For each  $j \in \{1, 2, ..., k\}$  a function  $T_j$  from  $\mathbb{N}^{k'} \times \mathbb{N}$  to  $\{0, 1\} \times \mathbb{N}$  mapping a variable assignment  $\overline{a}$  and a trace name n to a pair  $(b, \ell)$  where the bit b encodes whether the trace named n is in the set assigned to  $Y_j$  (w.r.t. the variable assignment encoded by  $\overline{a}$ ) and where the natural number  $\ell$  is intended to encode in which level of the fixed point computation the trace named n was added to the fixed point (computed with respect to  $\overline{a}$ ). That this is correct will be captured by the formula we are constructing.
- A function Sk from  $\mathbb{N} \times \mathbb{N}^*$  to  $\mathbb{N}$  to be interpreted as Skolem functions for the existentially quantified trace variables of  $\varphi$ , i.e., we map a variable name and a variable assignment of the variables preceding it to a trace name.
- A function E from  $\mathbb{N}^{k'} \times \mathbb{N} \times \mathbb{N}$  to  $\mathbb{N}$ , where, for a fixed  $\overline{a} \in \mathbb{N}^{k'}$  encoding a variable assignment  $\Pi$ , the function  $x, j \mapsto E(\overline{a}, x, j)$  is intended to encode the function  $e_{\varphi,\Pi}$ , i.e., x encodes a subformula in  $\Phi$  and j is a position. That this is correct will again be captured by the formula we are constructing.

Then, we express the following properties which characterize T being a model of  $\varphi$ :

- The function Sk is indeed a Skolem function for  $\varphi$ , i.e., for all variable assignments  $\overline{a} \in \mathbb{N}^{\ell}$ , if the traces assigned to universally quantified variables  $\pi$  are in the set  $X_{\pi}$  that  $\pi$  ranges over, then the traces assigned to the existentially quantified variables  $\pi'$  are in the set  $X_{\pi'}$  that  $\pi'$  ranges over. Note that  $X_{\pi}$  and  $X_{\pi'}$  can either be T or one of the  $Y_j$ , for which we can check membership via the functions  $T_j$ . Also note that this formula refers to traces by their names (which are natural numbers) and quantifies over variable assignments (which are encoded by natural numbers), i.e., it is a first-order formula.
- For every variable assignment  $\overline{a}$  such that the traces assigned to universally quantified variables  $\pi$  are in the set  $X_{\pi}$  that  $\pi$  ranges over and that is consistent with the Skolem functions encoded by Sk: the function  $x, j \mapsto E(\overline{a}, x, j)$  satisfies the consistency conditions characterising the expansion, and we have  $E(\overline{a}, x_0, 0) = 1$ , where  $x_0$  is the encoding of  $\psi$ . Again, this formula is first-order.
- For every variable assignment  $\overline{a}$  as above, the set assigned to  $Y_j$  by  $T_j$  w.r.t.  $\overline{a}$  is indeed the least fixed point of  $f_{\overline{a},j}$ . Here, we use the information about the stages encoded by  $T_j$  and again have to use the expansion E to check that the step formula is satisfied by the selected traces. As before, this can be done in first-order arithmetic.

We leave the tedious, but straightforward details to the reader.

## J Proof of Theorem 8

Recall that we need to show that lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> finite-state satisfiability and model-checking are both in  $\Sigma_2^2$  and  $\Sigma_1^1$ -hard and that the lower bound already holds for  $X_a$ -free sentences.

*Proof.* We show the upper bounds for arbitrary sentences (possibly using  $X_a$ ) and the lower bounds for  $X_a$ -free sentences (recall Remark 4).

We begin by considering finite-state satisfiability. Recall that  $\text{Hyper}^2 \text{LTL}_{fp}$ , and therefore also  $\text{lfp-Hyper}^2 \text{LTL}_{fp}$  can be translated into  $\text{Hyper}^2 \text{LTL}$  (see Proposition 2). The translation replaces every occurrence of a quantifier  $Q(Y, \gamma, \varphi^{\text{con}})$  in a  $\text{lfp-Hyper}^2 \text{LTL}_{fp}$  sentence  $\varphi$  by

$$\exists Y.\varphi^{\mathrm{con}} \land \forall Y'.(\varphi^{\mathrm{con}}[Y/Y'] \to \exists \pi \in Y'. \neg \pi \triangleright Y),$$

where  $\varphi^{\operatorname{con}}[Y/Y']$  is the formula obtained from  $\varphi^{\operatorname{con}}$  by replacing every occurrence of Y by Y'. Intuitively, the resulting formula expresses that Y must be interpreted by some smallest set (in the subset order) satisfying the guard  $\varphi^{\operatorname{con}}$ . Due to the monotonicity of the operator induced by the guard, this smallest set is unique and equal to the least fixed point. Now, a naive application of the translation introduces one quantifier alternation per translated least fixed point quantifier. However, this is not necessary: due to the restrictive second-order quantification, only over (unique) least fixed points, the second-order quantifiers can also be arranged so that the second-order quantification has an  $\exists^*\forall^*$ -pattern: The subformulas  $\forall Y'.(\varphi^{\operatorname{con}}[Y/Y'] \to \exists \pi \in Y'. \neg \pi \triangleright Y)$ are independent of each other and existential quantification of the sets Y does not depend on the universally quantified sets Y'. Hence, the universal quantification of the Y' can be moved behind the other existential set quantifiers.

Such Hyper<sup>2</sup>LTL sentences  $\varphi$  can be translated into sentences  $\varphi'$  of third-order arithmetic that capture finite-state satisfiability of  $\varphi$ . The third-order quantifiers of  $\varphi'$  has an  $\exists^*\forall^*$ -pattern as well: The translation adds two existential second-order quantifiers in the beginning, then the quantifier pattern of  $\varphi'$  follows that of  $\varphi$ . Hence, we obtain the desired  $\Sigma_2^2$  upper bound.

Now, let us show that the lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> finite-state satisfiability problem is  $\Sigma_1^1$ -hard (even for  $X_a$ -free sentences) by a reduction from a variant of the recurrent tiling problem, a standard  $\Sigma_1^1$ -complete problem [14].

A tile is a function  $\tau$ : {east, west, north, south}  $\to C$  that maps directions into a finite set C of colours. Given a finite set Ti of tiles, a tiling of the positive quadrant  $\mathbb{N} \times \mathbb{N}$  with Ti is a function  $ti: \mathbb{N} \times \mathbb{N} \to Ti$  with the property that for all  $i, j \in \mathbb{N}$ 

- ti(i, j)(east) = ti(i+1, j)(west), and
- ti(i, j)(north) = ti(i, j + 1)(south).

The recurrent tiling problem is to determine, given a finite set Ti of tiles and a designated  $\tau_0 \in Ti$ , whether there is a tiling ti of the positive quadrant with Ti such that  $\tau_0$  appears infinitely often in the bottom row, i.e., there are infinitely many i such that  $ti(i, 0) = \tau_0$ .

A tiling of the positive quadrant consists of infinitely many rows, each one being an infinite word over Ti. For our purposes, it would be much more convenient to work with a single trace encoding a whole tiling. A tiling of the whole positive quadrant can be mirrored along the diagonal  $\{(n,n) \mid n \in \mathbb{N}\}$ , yielding a tiling of the wedge  $W = \{(i, j \in \mathbb{N} \times \mathbb{N}) \mid i < j\}$  above the diagonal by product tiles (encoding a tiling of the wedge above the diagonal and a tiling of the wedge below (and including) the diagonal). This requires to mirror and rotate the tiles encoding the lower wedge as well as some straightforward modifications to deal with the diagonal itself.

Formally, a tiling of W with Ti is a function  $ti: W \to Ti$  with the property that for all  $i, j \in \mathbb{N}$ 

- if  $0 \le i < j 1$ , then ti(i, j)(east) = ti(i + 1, j)(west), and
- if i < j, then ti(i, j)(north) = ti(i, j + 1)(south).

The recurrent wedge tiling problem is to determine, given a finite set Ti of tiles and a designated subset  $Ti_0 \subseteq Ti$ , whether there is a tiling ti of the positive quadrant with Ti such that tiles from  $Ti_0$  appear infinitely often in the leftmost column, i.e., there are infinitely many j such that  $ti(0, j) \in Ti_0$ . For the sake of brevity, we call such a ti a  $(Ti, Ti_0)$ -tiling.

As sketched above, the recurrent wedge tiling problem is also  $\Sigma_1^1$ -hard, as we can reduce the recurrent tiling problem to it. Note that  $\tau_0$  appearing infinitely often in the bottom row in a tiling of the whole positive quadrant is captured by pairs of tiles with  $\tau_0$  in the first component appearing infinitely often in the leftmost column of a tiling of the wedge W (to which the bottom row is mirrored to). This is the reason we consider a set of designated tiles appearing infinitely often.

Now, a tiling  $ti: W \to Ti$  can be represented by a single infinite trace

 $\{ti(0,1)\}$  {#}  $\{ti(0,2)\}$  { $ti(1,2)\}$  {#}  $\{ti(0,3)\}$  { $ti(1,3)\}$  { $ti(2,3)\}$  {#} ...

over  $Ti \cup \{\#\}$  listing each row of ti up to the diagonal. In the following, we will often identify singleton subsets of  $Ti \cup \{\#\}$  with the element they contain.

Let us continue by explaining how to check, using  $lfp-Hyper^2LTL_{fp}$ , whether a set Ti admits a recurrent wedge tiling. Consider a word of the form

$$t = \{\tau_{0,1}\} \{\#\} \{\tau_{0,2}\} \{\tau_{1,2}\} \{\#\} \{\tau_{0,3}\} \{\tau_{1,3}\} \{\tau_{2,3}\} \{\#\} \cdots$$

Whether the encoded rows are horizontally compatible can be checked by inspecting adjacent letters of t. Similarly, whether infinitely many tiles from  $Ti_0$  appear in the first column can be checked by looking for infinitely many # being followed by a  $\{\tau\}$  with  $\tau \in Ti_0$ . Both checks can easily be implemented in LTL. It remains to consider vertical compatibility. Let

$$t_j = \{\tau_{0,j}\}\{\tau_{1,j}\}\cdots\{\tau_{j-1,j}\}\{\#\}\cdots$$

and

$$t_{j+1} = \{\tau_{0,j+1}\}\{\tau_{1,j+1}\}\cdots\{\tau_{j-1,j+1}\}\{\tau_{j,j+1}\}\{\#\}\cdots$$

be the suffixes of t starting with the j-th and (j + 1)-th rows, respectively. These two rows are vertically compatible if  $\tau_{i,j}(\text{north}) = \tau_{i,j+1}(\text{south})$  for all i < j. Furthermore, these two suffixes also let us verify that the (j + 1)-th row has one more tile than the j-th row. Both checks are implementable in quantifier-free HyperLTL with a formula having two free variables for the two suffixes.

Intuitively, we will write a formula that expresses the existence of a trace  $t_c$  (tentatively encoding a tiling), then use a fixed point to compute the set of suffixes of  $t_c$ , and then require that  $t_c$  is horizontally

compatible and contains infinitely many tiles from  $Ti_0$  after #'s. Further, we require that, for all  $j \in \mathbb{N}$ , the suffix  $s_j$  of  $t_c$  starting after the *j*-th # and the suffix  $s_{j+1}$  of  $t_c$  starting after the (j+1)-th # are vertically compatible up to the first # in  $s_j$ , as well as that  $s_{j+1}$  has then one more tile and then a #. The set of suffixes is obtained by removing the first letter from a trace that is already in the fixed point, starting with  $t_c$ . The minimality constraint takes care of only suffixes of  $t_c$  being in the fixed point.

There is one last detail we need to explain: How to identify  $s_j$ ? Note that we actually only have to pair  $s_j$  with  $s_{j+1}$  for all j. We do so by "marking" a unique position of each trace in the fixed point so that a trace has its mark at position j if and only if it has been obtained by removing j #'s. Several suffixes may have their mark at the same position, e.g.,

$$\{\tau_{0,j}\}\{\tau_{1,j}\}\cdots\{\tau_{j-1,j}\}\{\#\}\cdots$$

and

$$\{\tau_{1,j}\}\cdots\{\tau_{j-1,j}\}\{\#\}\cdots$$

are both obtained removing j - 1 many #'s. However, ultimately, we are only interested in suffixes that start right after a #, all others are in the fixed point only because we have to "compute" the suffixes by removing one letter at a time. Hence, the proposition we use to mark traces comes in two forms:  $\mathbf{x}$  and  $\mathbf{x}^{\#}$  where the later signifies that this trace is obtained by removing a #. We show that this process of taking and comparing suffixes can proceed indefinitely if and only if the trace we started with encodes a recurrent wedge tiling.

Let Ti be finite a set of tiles and let  $Ti_0 \subseteq Ti$ . We, fix  $AP = Ti \cup \{\#, \mathbf{x}, \mathbf{x}^{\#}\}$  and express the existence of a  $(Ti, Ti_0)$ -tiling by the lfp-Hyper<sup>2</sup>LTL<sub>fp</sub> sentence

$$\varphi_{Ti,Ti_0} = \varphi_m \land \exists \pi_c \in X_d. \left( \varphi_c(\pi_c) \land \exists (Y, \curlyvee, \varphi^{\operatorname{con}}(\pi_c, Y)). \varphi_{\operatorname{inf}}(Y) \land \varphi_{\operatorname{vrt}}(Y) \right)$$

with the following subformulas:

- $\varphi_m$  expresses the following constraints on traces in the model:
  - Exactly one of the propositions in  $Ti \cup \{\#\}$  holds at any position.
  - There are infinitely many #, but no two in a row. This implies that each trace encodes an infinite sequence of finite nonempty words over Ti.
  - Each of these words is horizontally consistent.
  - Either x holds at most once, or x<sup>#</sup> holds at most once, but not both of them.<sup>4</sup>

$$\varphi_{m} = \forall \pi \in X_{d}. \quad \mathbf{G}(\bigvee_{\mathbf{p} \in T_{i} \cup \{\#\}} (\mathbf{p}_{\pi} \land \bigwedge_{\mathbf{p}' \in (T_{i} \cup \{\#\}) \setminus \{\mathbf{p}\}} \neg \mathbf{p}'_{\pi})) \land$$
$$\mathbf{G} \mathbf{F} \#_{\pi} \land \neg \mathbf{F}(\#_{\pi} \land \mathbf{X} \#_{\pi}) \land$$
$$\mathbf{G}(\bigvee_{\tau \in T_{i}} \tau_{\pi} \to (\#_{\pi} \lor \bigvee_{\substack{\tau' \in T_{i} \\ \tau(\text{west}) = \tau'(\text{east})}} \mathbf{X} \tau'_{\pi}) \land$$
$$(\neg \mathbf{x}_{\pi} \land \neg \mathbf{x}_{\pi}^{\#}) \mathbf{U}((\mathbf{x}_{\pi} \oplus \mathbf{x}_{\pi}^{\#}) \land \mathbf{X} \mathbf{G}(\neg \mathbf{x}_{\pi} \land \neg \mathbf{x}_{\pi}^{\#}))$$

•  $\varphi_c(\pi_c) = \mathbf{x}_{\pi_c}^* \wedge \mathbf{G} \mathbf{F} \bigvee_{\tau \in Ti_0} (\#_{\pi_c} \wedge \mathbf{X} \tau_{\pi_c})$  expresses that  $\mathbf{x}^*$  appears at position 0 of the trace  $t_c$  assigned to  $\pi_c$  (i.e., it is one of the traces used to check vertical compatibility) and that tiles from  $Ti_0$  appear infinitely often in  $t_c$  after #'s. Note that  $t_c$  is a trace of the model and therefore satisfies all the requirements expressed by  $\varphi_m$ . We use  $t_c$  as seed for the fixed point assigned to Y.

<sup>&</sup>lt;sup>4</sup>Recall that the set Tr of traces of a finite transition system is closed. Thus, if it contains all traces that have exactly one x (one  $x^*$ ), it must also contain traces that do not have a x ( $x^*$ ).

- $\varphi^{\text{con}}(\pi_c, Y)$  expresses that for all traces t already in the fixed point (and thus also from the model) and all traces t' in the model (so both satisfy the requirements expressed in  $\varphi_m$ ),
  - if t is marked by a  $\mathbf{x}^{\#}$  and t' is the unique trace obtained from the  $(Ti \cup \{\#\})$ -projection of t by removing the first letter and adding x at the same position as  $\mathbf{x}^{\#}$  in t, or
  - if t is marked by a x, does not start with #, and t' is the unique trace obtained from the  $(Ti \cup \{\#\})$ projection of t by removing the first letter (which is not a #) and adding x at the same position
    as x in t, or
  - if t is marked by a x, starts with #, and t' is the unique trace obtained from the  $(Ti \cup \{\#\})$ projection of t by removing the first letter (which is a #) and adding x<sup>#</sup> one position after the
    position where t has the x,

then t' is also in the fixed point.

$$\varphi^{\operatorname{con}}(\pi_{c}, Y) = \pi_{c} \triangleright Y \land \forall \ddot{\pi} \in Y. \ \forall \ddot{\pi}' \in X_{d}. \ \ddot{\pi}' \triangleright Y \leftarrow \left[ \left( \mathbf{F} \, \mathbf{x}_{\pi}^{\#} \land \varphi_{\operatorname{shft}}(\pi, \pi') \land \mathbf{G}(\mathbf{x}_{\pi}^{\#} \leftrightarrow \mathbf{x}_{\pi'}) \right) \lor \right. \\ \left. \left( \mathbf{F} \, \mathbf{x}_{\pi} \land \neg \#_{\pi} \land \varphi_{\operatorname{shft}}(\pi, \pi') \land \mathbf{G}(\mathbf{x}_{\pi} \leftrightarrow \mathbf{x}_{\pi'}) \right) \lor \right. \\ \left. \left( \mathbf{F} \, \mathbf{x}_{\pi} \land \#_{\pi} \land \varphi_{\operatorname{shft}}(\pi, \pi') \land \mathbf{G}(\mathbf{x}_{\pi} \leftrightarrow \mathbf{X} \, \mathbf{x}_{\pi'}^{\#}) \right) \right] \right]$$

with

$$\varphi_{\rm shft}(\pi,\pi') = \mathbf{G} \bigwedge_{\mathbf{p}\in Ti\cup\{\#\}} ((\mathbf{X}\,\mathbf{p}_{\pi})\leftrightarrow\mathbf{p}_{\pi'})$$

This adds for each trace t already in the fixed point at most one trace to the fixed point, namely the unique trace t' described above (provided it is in the model).

The position of the mark  $\mathbf{x}/\mathbf{x}^{\#}$  does keep track of how many # have been removed from  $t_c$  and that a trace in the (least) fixed point is marked by  $\mathbf{x}^{\#}$  if and only if it is obtained by removing a #.

- $\varphi_{\inf}(Y) = \forall \pi \in Y$ .  $\exists \pi' \in Y$ .  $\mathbf{F}(\mathbf{x}_{\pi}^{\#} \wedge \mathbf{X} \mathbf{x}_{\pi'}^{\#})$  expresses that for each trace t in the least fixed point marked with  $\mathbf{x}^{\#}$  (say at position j), there is another trace t' in the least fixed point that is marked with  $\mathbf{x}^{\#}$  at position j + 1. As  $t_c$ , which is marked with  $\mathbf{x}^{\#}$  at position 0, is in the fixed point, this implies that the fixed point contains such a trace for every j. This in particular implies that the fixed point terminate prematurely, i.e., the fixed point contains all suffixes of  $t_c$  (with correct marks, as explained above).
- $\varphi_{\text{vrt}}$  expresses the vertical compatibility requirement: for all traces t, t' in the least fixed point, if both are marked by  $\mathbf{x}^{\#}$  (at some position j in t and position j + 1 in t'), then their tiles are vertically compatible (t' above t) up to the first # in t. At that position, t' must have another tile and then a #.

$$\forall \pi \in Y. \ \forall \pi' \in Y. \ \mathbf{F}(\mathbf{x}_{\pi}^{\#} \wedge \mathbf{X} \ \mathbf{x}_{\pi'}^{\#}) \rightarrow \left(\bigvee_{\substack{\tau, \tau' \in Ti \\ \tau(\text{north}) = \tau'(\text{south})}} \tau_{\pi} \wedge \tau_{\pi'}'\right) \mathbf{U}(\#_{\pi} \wedge \neg \#_{\pi'} \wedge \mathbf{X} \ \#_{\pi'})$$

As usual,  $\varphi_{Ti,Ti_0}$  can be brought into prenex normal form.

We show that  $\varphi_{Ti,Ti_0}$  is satisfied by a finite transition system if and only if there is a  $(Ti, Ti_0)$ -tiling.

So, let  $\varphi_{T_i,T_{i_0}}$  be satisfied by  $T = \text{Tr}(\mathfrak{T})$  for some finite transition system  $\mathfrak{T}$ . In particular, all traces in T satisfy the requirements expressed by  $\varphi_m$ . Also, there is a  $t_c \in T$  satisfying all requirements expressed by  $\varphi_c$ . Thus,  $t_c$  must have the form (ignoring the marks  $\mathbf{x}, \mathbf{x}^{\#}$ )

$$t = r_0 \{\#\} r_1 \{\#\} r_2 \{\#\} \cdots$$

where each  $r_j$  is a finite nonempty word of horizontally compatible tiles and infinitely many  $r_j$  start with a tile from  $Ti_0$ .

Furthermore, there is an  $S \subseteq T$  such that S is the least fixed point of the function induced by  $\varphi^{\text{con}}$  w.r.t. the variable assignment  $\{X_d \mapsto T, \pi_c \mapsto t_c\}$  and

$$\{X_d \mapsto T, \pi_c \mapsto t_c, Y \mapsto S\} \models \varphi_{\inf} \land \varphi_{vrt}$$

Let us first consider S: as argued above, for every trace in S, one additional trace gets added to S by  $\varphi^{\text{con}}$ , as the fixed point must be infinite due to the subformula  $\varphi_{\text{inf}}$ . Hence, we obtain a sequence  $t_0, t_1, t_2, \ldots$  of traces starting with  $t_0 = t_c$  such that  $S = \{t_j \mid j \in \mathbb{N}\}$  and  $\{\ddot{\pi} \mapsto t_j, \ddot{\pi}' \mapsto t_{j+1}\}$  satisfies the subformula

$$\begin{pmatrix} \mathbf{F} \mathbf{x}_{\pi}^{\texttt{\#}} \land \varphi_{\mathrm{shft}}(\pi, \pi') \land \mathbf{G}(\mathbf{x}_{\pi}^{\texttt{\#}} \leftrightarrow \mathbf{x}_{\pi'}) \end{pmatrix} \lor \\ \begin{pmatrix} \mathbf{F} \mathbf{x}_{\pi} \land \neg \#_{\pi} \land \varphi_{\mathrm{shft}}(\pi, \pi') \land \mathbf{G}(\mathbf{x}_{\pi} \leftrightarrow \mathbf{x}_{\pi'}) \end{pmatrix} \lor \\ \begin{pmatrix} \mathbf{F} \mathbf{x}_{\pi} \land \#_{\pi} \land \varphi_{\mathrm{shft}}(\pi, \pi') \land \mathbf{G}(\mathbf{x}_{\pi} \leftrightarrow \mathbf{X} \mathbf{x}_{\pi'}^{\texttt{\#}}) \end{pmatrix}$$

of  $\varphi^{\text{con}}$ . Thus,  $t_{j+1}$  is obtained from  $t_j$  removing the first letter and updating the mark so that it counts the number of #'s that were removed so far. Hence,  $t_j$  is the suffix of  $t_c$  obtained by removing the first j letters (again ignoring the marks).

Now, as  $\varphi_{\text{vrt}}$  is satisfied and the marks are moved correctly, we can conclude that  $|r_j| + 1 = |r_{j+1}|$  and  $r_j$  and  $r_{j+1}$  are vertically compatible. Thus, the  $r_j$  can be arranged into a wedge tiling, which is recurrent as infinitely many  $r_j$  start with a tile from  $Ti_0$ .

Conversely, assume there is a  $(Ti, Ti_0)$ -tiling ti. Let  $\mathfrak{T}_{Ti}$  be a finite transition system whose set T of traces contains exactly the traces whose  $(Ti \cup \{\#\})$ -projection is of the form

$$r_0 \{\#\} r_1 \{\#\} r_2 \{\#\} \cdots$$

where each  $r_j$  is a nonempty finite word of tiles and where at most one position is marked with either **x** or  $\mathbf{x}^{\#}$ . We claim that  $T \models \varphi_{Ti, Ti_0}$ . To this end, let

$$t_c = \{ti(0,1), \mathbf{x}^{\#}\} \{\#\} \{ti(0,2)\} \{ti(1,2)\} \{\#\} \{ti(0,3)\} \{ti(1,3)\} \{ti(2,3)\} \{\#\} \dots \in T\}$$

and define the set  $S = \{t_0, t_1, t_2, \ldots\}$  via  $t_0 = t_c$  and, for j > 0

$$t_{j}(n) = \begin{cases} t_{c}(n+j) \cap (Ti \cup \{\#\}) \cup \{\mathbf{x}\} & \text{if } n \text{ is the number of } \# \text{ in } t_{c}(0) \dots t_{c}(j-1) \\ & \text{and } t_{c}(j-1) \neq \#, \\ t_{c}(n+j) \cap (Ti \cup \{\#\}) \cup \{\mathbf{x}^{\#}\} & \text{if } n-1 \text{ is the number of } \# \text{ in } t_{c}(0) \dots t_{c}(j-1) \\ & \text{and } t_{c}(j-1) = \#, \\ t_{c}(n+j) \cap (Ti \cup \{\#\}) & \text{otherwise.} \end{cases}$$

Each  $t_i$  is in T.

Now, we have  $\{X_d \mapsto T\} \models \varphi_m, \Pi = \{X_d \mapsto T, \pi_c \mapsto t_c\} \models \varphi_c, S$  is equal to the least fixed point induced by  $\varphi^{\text{con}}$  w.r.t.  $\Pi$ , and  $\Pi[Y \mapsto S] \models \varphi_{\text{inf}} \land \varphi_{\text{vrt}}$ . This shows that we indeed have  $\mathfrak{T} \models \varphi_{Ti, Ti_0}$  as required.

Finally, let us consider model-checking. Our approach to the upper bound is inspired by the similar construction for Hyper<sup>2</sup>LTL model-checking (see the proof of Theorem 4): Instead of existentially quantifying a finite-transition system in the formula we have constructed above to place the finite-state satisfiability problem in  $\Sigma_{2}^{2}$ , we hardcode the given transition system to be model-checked into the formula.

For the lower bound we rely on the reduction from tiling to finite-state satisfiability: The transition system  $\mathfrak{T}_{Ti}$  satisfies  $\varphi_{Ti,Ti_0}$  if and only if there is a recurrent wedge tiling ti with Ti and  $Ti_0$ . Thus, model-checking is indeed  $\Sigma_1^1$ -hard.