# Existential Calculi of Relations with Transitive Closure: Complexity and Edge Saturations

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Abstract—We study the decidability and complexity of equational theories of the existential calculus of relations with transitive closure (ECoR\*) and its fragments, where ECoR\* is the positive calculus of relations with transitive closure extended with complements of term variables and constants. We give characterizations of these equational theories by using edge saturations and we show that the equational theory is 1) coNP-complete for ECoR\* without transitive closure; 2) in coNEXP for ECoR\* without intersection and PSPACE-complete for two smaller fragments; 3)  $\Pi_1^0$ -complete for ECoR\*. The second result gives PSPACE-upper bounds for some extensions of Kleene algebra, including Kleene algebra with top w.r.t. binary relations.

Index Terms-relation algebra, Kleene algebra, complexity

#### I. INTRODUCTION

The calculus of relations (CoR, for short) [1] is an algebraic system on binary relations. As binary relations appear everywhere in computer science, CoR and relation algebras (including their transitive closure extensions) can be applied to various areas, such as databases and program development and verification. However, the equational theory of CoR is *undecidable* [2]. The undecidability holds even over the signature  $\{\cdot, \cup, \_^-\}$  of composition  $(\cdot)$ , union  $(\cup)$ , and complement  $(\_^-)$  [3, Thm. 1], moreover even when the number of term variables is one [4].

One approach to avoid the undecidability of the equational theory of CoR is to consider its *positive* fragments, by excluding complements. The terms of *the positive calculus of relations* (PCoR, for short) [5], [6] is the set of terms over the signature  $\{\cdot, \cup, \_, \bot, \top, I, \cap\}$  of composition  $(\cdot)$ , union  $(\cup)$ , converse  $(\_)$ , the empty relation  $(\bot)$ , the universal relation  $(\top)$ , the identity relation (I), and intersection  $(\cap)$ . The equational theory of PCoR is *decidable* [5]. This decidability result also holds when adding the reflexive transitive operator, thus arriving at Kleene allegory terms [7]–[9].

Then, it is natural to ask about the decidability and complexity of PCoR when the complement operator is added in restricted ways (cf. e.g., antidomain [10], [11] and tests in Kleene algebra with tests (KAT) [12]) to extend the expressive power of PCoR without drastically increasing the complexity. In this paper, inspired by the negations of atomic programs in the context of propositional dynamic logic (PDL) [13]–[15], we consider existential calculi of relations—positive calculi of relations extended with complements of term variables and constants (i.e., the complement operator only applies

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to term variables or constants)—and study the decidability and complexity of their equational theories. We denote by PCoR\* the PCoR with the reflexive transitive closure operator (\_\*). We denote by ECoR (resp. ECoR\*) the PCoR (resp. PCoR\*) with complements of term variables and constants. For example, whereas  $(a \cdot a)^-$  and  $(a^*)^-$  are not ECoR terms, ECoR contains terms such as:

$$\begin{array}{c} a^- \\ (a \cdot a) \cap a^- \cap \mathsf{I}^- \end{array} \qquad \left( \begin{array}{c} \text{there is } not \text{ an } (a\text{-labeled}) \text{ edge} \\ \text{from the source to the target} \\ \text{the distance from the source} \\ \text{to the target is two} \end{array} \right)$$

They are not expressible in PCoR because they are not preserved under homomorphisms; thus, ECoR is strictly more expressive than PCoR. More precisely, w.r.t. binary relations, while PCoR has the same expressive power as the three-variable fragment of *existential positive* logic with equality [16, Cor. 3.2], ECoR has the same expressive power as the three-variable fragment of *existential* logic with equality [16, Cor. 3.14]<sup>1</sup>. (The name "*existential* calculi of relations" comes from this fact.)

On the equational theory of ECoR\*, while it subsumes that of PCoR\* (including axioms of Kleene algebra and allegory [6]), some non-trivial valid (in)equations are as follows (see Appendix A for the proofs):

$$T = a \cup a^{-} \tag{1}$$
  $a \le I^{-} \cup aa \tag{3}$ 

$$aba^- < I^-a^- \cup aI^-$$
 (2)  $a^-a^- < I^-$  (4)

Contribution and related work

We show that the equational theory is

- 1) coNP-complete for ECoR (Thm. 24);
- 2) in coNEXP for ECoR without ∩ (Thm. 35); PSPACE-complete for ECoR without ∩ such that I<sup>-</sup> does not occur (Thm. 41) and for ECoR without ∩ such that a<sup>-</sup> does not occur for any term variable a (Thm. 44);
- 3)  $\Pi_1^0$ -complete for ECoR\* (Thm. 50).

Table I summarizes our results and related results. 2) gives PSPACE-upper bounds for some extensions of *Kleene algebra* 

 $^1\text{ECoR}$  has the same expressive power as the level  $\Sigma_1^{\text{CoR}}$  of the dot-dagger alternation hierarchy [17] [16, Def. 3.13] of CoR, because every ECoR term is a  $\Sigma_1^{\text{CoR}}$  term, and conversely, every  $\Sigma_1^{\text{CoR}}$  term has an equivalent ECoR term by pushing complement and projection deeper into the term to the extent possible. Here,  $\Sigma_1^{\text{CoR}}$  has the same expressive power as the three-variable fragment of existential logic (i.e., the level  $\Sigma_1$  of the quantifier alternation hierarchy of first-order logic) [16, Cor. 3.14].

Complexity of the equational theory (w.r.t. binary relations) over  $S \cup S'$  where  $S \subseteq \{\cdot, \cup, \_{}^{\smile}, \cap, \_*, \bot, \top, I\} = S_{PCoR*}$  and  $S' \subseteq \{a^-, I^-, \_^-\}$ . Here,  $a^-, I^-, \_^-$  denote the complements of term variables, those of constants, and the (full) complement.

$S \longrightarrow S'$	Ø	{I <sup>-</sup> }	$\{a^{-}\}$	$\{a^-,I^-\}$	{}
$\{\cdot, \cup\} \subseteq S \subseteq S_{PCoR*} \setminus \{\_*\}$	coNP-c ([18], [19], [3, Lem. 8])	(	coNP-c Thm. 24)		$\Sigma_1^0$ -c ([1]–[3])
$\{\cdot, \cup, \_^*\} \subseteq S \subseteq S_{PCoR*} \setminus \{\cap\}$	PSPACE-c ([18], [19], Thm. 41)	PSPACE-c (Thm. 44)	PSPACE-c (Thm. 41)	in coNEXP (Thm. 35)	$\Pi_1^1$ -c
$\{\cdot, \cup, \cap, \_^*\} \subseteq S \subseteq S_{PCoR*}$	EXPSPACE-c ([7]–[9])	EXPSPACE-hard [8], [9]	П <sub>1</sub> <sup>0</sup> -с (Thm. 50)		([20, p.332], [15] <sup>2</sup> )

(KA) w.r.t. binary relations, as ECoR without  $\cap$  includes KA terms (i.e., terms over the signature  $\{\cdot, \cup, \_^*, \bot, I\}$ ). Notably, it includes KA with converse ( $\smile$ ) [22], [23] and KA with top ( $\top$ ) [24] w.r.t. binary relations; thus, the result gives a positive answer to a question posed by Pous and Wagemaker [24, p. 14] as follows: the equational theory of KA with top w.r.t. binary relations is still in PSPACE.<sup>3</sup> Additionally, 3) negatively answers a question posed by Nakamura [9, p. 12] as follows: the equational theory of Kleene allegories with complements of term variables (w.r.t. binary relations) is undecidable.

To show them, we give a graph theoretical characterization of the equational theory of ECoR\* (Sect. IV). The characterization using graph languages and graph homomorphisms is based on that for PCoR\*, by Brunet and Pous [8, Thm. 3.9][6, Thm. 16], but the identical characterization fails for ECoR\*. Nevertheless, we can extend such a characterization even for ECoR\*, by extending their graph languages, using edge saturations (cf. saturations of graphs [26], [27]; in our saturation, the vertex set is fixed). Using this graph characterization, we can show the upper bounds of 1) and 3).

For the upper bound of 2): the equational theory of ECoR\* without intersection, we refine the graph characterization above by using path graphs with some additional information, called *saturable paths* (Sect. V). This notion is inspired by Hintikka-trees for Boolean modal logics [13] and PDL with the negation of atomic programs [14], where we consider paths instead of infinite trees and introduce the converse and the difference relation  $I^-$ . This characterization gives the coNEXP upper bound for the equational theory of ECoR\* without intersection. Moreover, for some fragments, we can give *word automata* using saturable paths, which shows that the equational theory of ECoR\* without intersection is decidable in PSPACE if  $I^-$  does not occur (Thm. 41) or if  $a^-$  does not occur (for any term variable a) (Thm. 44). (Our automata construction cannot apply to the full case (Remark 45).)

For the lower bounds, 1) and 2) are immediate from the results known in regular expressions [18], [19]. For 3), we give a reduction from the universality problem for context-free grammars (Sect. VI), via KA with hypotheses [28]–[30]

of the form  $t \le a$  (where t is a term and a is a term variable) w.r.t. binary relations.

#### Outline

Sect. II briefly gives basic definitions. Sect. III defines ECoR\* (Sect. III-A) and recalls known results w.r.t. word and graph languages for smaller fragments of ECoR\* (Sects. III-B, III-C). In Sect. IV, we give a graph theoretical characterization for ECoR\*, using *edge saturations*. By using this, we prove 1) and the upper bound of 3). In Sect. V, we introduce *saturable paths*, which refine the characterization of graph saturations, for ECoR\* without intersection. Moreover, we give automata using saturable paths for two smaller fragments. By using them, we prove 2). In Sect. VI, we prove the lower bound of 3). Sect. VII concludes this paper.

#### II. PRELIMINARIES

We write  $\mathbb N$  for the set of all non-negative integers. For  $l,r\in\mathbb N$ , we write [l,r] for the set  $\{i\in\mathbb N\mid l\le i\le r\}$ . For  $n\in\mathbb N$ , we write [n] for [1,n]. For a set A, we write #(A) for the cardinality of A and  $\wp(A)$  for the power set of A.

# A. Graphs

For  $k \in \mathbb{N}$ , a k-pointed graph G over a set A is a tuple  $\langle |G|, \{a^G\}_{a \in A}, 1^G, \dots, k^G \rangle$ , where

- |G| is a non-empty set of *vertices*;
- $a^G \subseteq |G|^2$  is a binary relation for each  $a \in A$  ( $\langle x, y \rangle \in a^G$  denotes that there is an a-labeled edge from x to y);
- $1^G, \ldots, k^G \in |G|$  are the vertices pointed by  $1, \ldots, k$ .

We say that 2-pointed graphs are graphs, here; we mainly use them. For 2-pointed graph G, we say that  $1^G$  and  $2^G$  are the *source* and target, respectively.

A (graph) homomorphism from a graph G to a graph H is a map h from |G| to |H| such that

- $\langle h(1^G), h(2^G) \rangle = \langle 1^H, 2^H \rangle;$
- $\langle h(x), h(y) \rangle \in a^H$  for every  $a \in A$  and  $\langle x, y \rangle \in a^G$ .

In particular, we say that h is isomorphism if h is bijective and  $\langle h(x), h(y) \rangle \not\in a^H$  for every  $a \in A$  and  $\langle x, y \rangle \not\in a^G$ . We write  $h \colon G \longrightarrow H$  if h is a homomorphism from G to H and write  $G \longrightarrow H$  if  $h \colon G \longrightarrow H$  for some h. The relation  $\longrightarrow$  is a preorder. We display graphs in a standard way, where the node having an ingoing (resp. outgoing) unlabeled arrow denotes the source (resp. the target). For example, the following are two connected graphs, and dotted arrows induce a homomorphism

between them: 
$$0 - b^{n}$$

 $<sup>^2</sup>$ On the lower bound, the validity problem for PDL with intersection and negation of atomic programs, which is  $\Pi^1_1$ -complete [15], is recursively reducible to the equational theory over the signature  $\{\cup,\cdot,\_^*,\_^-\}$  by the standard translation from modal logics to CoR [21, p. 95] while eliminating the identity using a fresh variable preserving the validity [4, Lem. 9].

<sup>&</sup>lt;sup>3</sup>Very recently, this result is also given in [25].

#### III. EXISTENTIAL CALCULI OF RELATIONS

A. The existential calculus of relations with transitive closure (ECoR\*): syntax and semantics

1) Syntax: We fix a finite set  $\Sigma$  of variables. The set of ECoR\* terms over  $\Sigma$  is defined as follows:<sup>4</sup>

$$\begin{split} \mathsf{ECoR} * \ni t, s, u &:= a \mid a^- \mid a^- \mid (a^-)^- \mid \mathsf{I} \mid \mathsf{I}^- \mid \bot \mid \top \\ &\mid t \cdot s \mid t \cup s \mid t \cap s \mid t^* \end{split} \qquad (a \in \Sigma) \end{split}$$

We use parentheses in ambiguous situations. We often abbrevi-

ate  $t \cdot s$  to ts. For  $n \in \mathbb{N}$ , we write  $t^n$  for  $\begin{cases} t \cdot t^{n-1} & (n \geq 1) \\ \mathsf{I} & (n = 0) \end{cases}$ . Let  $S_{\mathsf{ECoR}*} \triangleq \{\cdot, \cup, \_{}^{\smile}, \cap, \_{}^{\ast}, \bot, \top, \mathsf{I}\} \cup \{a^-, \mathsf{I}^-\}$ . Here, "\_ $\smile$ " only applies to a or  $a^-$  (for simplicity) and we use " $a^-$ " to denote the complement of term variables and "I-" to denote the complement of constants (the important complemented constant is only I<sup>-</sup> in this setting).

For  $S \subseteq S_{\mathsf{ECoR}*}$ , we write  $\mathcal{T}_S$  for the set of all terms t in ECoR\* s.t. every operator occurring in t matches one of S. We use the following acronyms for some signatures (recall the acronyms in Sect. I; here, extended KA (ExKA) terms are used to denote ECoR\* terms without  $\cap$ , in this paper):

$S_{acronym}$	operator set		
ECoR*	$\{\cdot, \cup, \_{}^{\smile}, \cap, \_^*, \bot, \top, I, a^-, I^-\}$		
ECoR	$S_{\text{ECoR}*} \setminus \{\_^*\}$		
ExKA	$S_{\text{ECoR}*} \setminus \{\cap\}  (= S_{\text{KA}} \cup \{\_, \top, a^-, I^-\})$		
PCoR*	$S_{ ext{ECoR}*} \setminus \{a^-, I^-\}$		
PCoR	$S_{PCoR*} \setminus \{\_^*\}$		
KA	$S_{PCoR*} \setminus \{\_{\smile}, \cap, \top\}  (= \{\cdot, \cup, \_*, \bot, I\})$		

Let  $\Sigma_{\mathsf{I}} \triangleq \Sigma \cup \{\mathsf{I}\}$  and let

$$\Sigma^{(-)} \triangleq \{a, a^- \mid a \in \Sigma\}; \qquad \Sigma_{\mathsf{I}}^{(-)} \triangleq \{a, a^- \mid a \in \Sigma_{\mathsf{I}}\}.$$

For each term  $t \in \Sigma_{\mathrm{I}}^{(-)} \cup \{\bot, \top\}, \ \bar{t}$  denotes the following

$$\overline{a} \triangleq a^-$$
:  $\overline{a^-} \triangleq a$ :  $\overline{I} \triangleq I^-$ :  $\overline{I^-} \triangleq I$ :  $\overline{\bot} \triangleq \top$ :  $\overline{\top} \triangleq \bot$ .

An equation t = s is a pair of terms. An inequation t < sis an abbreviation of the equation  $t \cup s = s$ .<sup>5</sup>

The size ||t|| of a term t is the number of symbols occurring in t. Also, let  $||t = s|| \triangleq ||t|| + ||s||$ .

2) Relational semantics: For binary relations R, Q on a set W, the relational converse  $R^{\smile}$ , the relational composition  $R \cdot Q$ , the *n*-th iteration  $R^n$  (where  $n \in \mathbb{N}$ ), and the reflexive transitive closure  $R^*$  are defined by:

$$R^{\smile} \triangleq \{ \langle y, x \rangle \mid \langle x, y \rangle \in R \}$$

$$R \cdot Q \triangleq \{ \langle x, z \rangle \mid \exists y \in W. \ \langle x, y \rangle \in R \ \land \ \langle y, z \rangle \in Q \}$$

$$R^{n} \triangleq \begin{cases} R \cdot R^{n-1} & (n \ge 1) \\ \{ \langle x, x \rangle \mid x \in W \} & (n = 0) \end{cases}; \quad R^{*} \triangleq \bigcup_{n \in \mathbb{N}} R^{n}.$$

<sup>4</sup>For simplicity, in the term set, the converse only applies to terms of the form a or  $a^-$  and  $\perp^-$  and  $\perp^-$  does not occur, but we can give a polynomialtime transformation to the term set (Appendix B) by taking the *converse* normal form and that  $\models_{\text{REL}} \bot^- = \top$  and  $\models_{\text{REL}} \top^- = \bot$  hold. Thus, our complexity upper bounds hold (Thms. 24, 41, 44, 50) even if we exclude these restrictions.

<sup>5</sup>Note that  $[t]_{\mathfrak{A}} \subseteq [s]_{\mathfrak{A}} \iff [t \cup s]_{\mathfrak{A}} = [s]_{\mathfrak{A}}$ .

**Definition 1.** We say that G is a k-pointed structure if G is a k-pointed graph over  $\Sigma_{1}^{(-)}$  such that

• 
$$I^G = \{\langle x, x \rangle \mid x \in |G|\};$$

• 
$$I^G = \{\langle x, x \rangle \mid x \in |G|\};$$
  
•  $\overline{a}^G = |G|^2 \setminus a^G \text{ for } a \in \Sigma_1.^6$ 

We say that 0-pointed structures are *structures*. We use  $\mathfrak{A}$ and  $\mathfrak{A}$  to denote 0- and 2-pointed structures, respectively. For a structure  $\mathfrak{A}$  and two vertices  $x, y \in |\mathfrak{A}|$ , we write  $\mathfrak{A}[x, y]$  for the 2-pointed structure  $\langle |\mathfrak{A}|, \{a^{\mathfrak{A}}\}_{a \in \Sigma^{(-)}}, x, y \rangle$ .

The binary relation  $[t]_{\mathfrak{A}} \subseteq |\mathfrak{A}|^2$  of an ECoR\* term t on a structure  $\mathfrak{A}$  is defined as follows (where  $a \in \Sigma$ ):

$$\begin{bmatrix} a \end{bmatrix}_{\mathfrak{A}} \triangleq a^{\mathfrak{A}} & \begin{bmatrix} a^{-} \end{bmatrix}_{\mathfrak{A}} \triangleq (a^{-})^{\mathfrak{A}} \\
 \begin{bmatrix} \bot \end{bmatrix}_{\mathfrak{A}} \triangleq \emptyset & \begin{bmatrix} \top \end{bmatrix}_{\mathfrak{A}} \triangleq |\mathfrak{A}|^{2} \\
 \begin{bmatrix} t \cup s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cup [s]_{\mathfrak{A}} & \begin{bmatrix} t \cap s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cap [s]_{\mathfrak{A}} \\
 \begin{bmatrix} \mathbb{I} \end{bmatrix}_{\mathfrak{A}} \triangleq \mathbb{I}^{\mathfrak{A}} & \begin{bmatrix} \mathbb{I} \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cap [s]_{\mathfrak{A}} \\
 \begin{bmatrix} t \cdot s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I} \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} \\
 \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} \\
 \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} \\
 \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} = [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} \\
 \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} \\
 \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} & \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} & \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} & \begin{bmatrix} \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} & \mathbb{I}^{*} \end{bmatrix}_{\mathfrak{A}} &$$

We write  $\models_{\text{REL}} t = s$  if  $[\![t]\!]_{\mathfrak{A}} = [\![s]\!]_{\mathfrak{A}}$  for every structure  $\mathfrak{A}$ . The equational theory over S w.r.t. binary relations is defined as the set of all pairs t = s of terms in  $\mathcal{T}_S$  s.t.  $\models_{REL} t = s$ .

**Notation 2.** Based on  $[\![\ ]\!]_{\mathfrak{A}}$ , we define the following notations:

$$\begin{split} &\mathfrak{A}[x,y] \models t \iff \langle x,y \rangle \in [\![t]\!]_{\mathfrak{A}} \\ &\ddot{\mathfrak{A}} \models t = s \iff (\ddot{\mathfrak{A}} \models t) \leftrightarrow (\ddot{\mathfrak{A}} \models s) \\ &\mathfrak{A} \models t = s \iff [\![t]\!]_{\mathfrak{A}} = [\![s]\!]_{\mathfrak{A}}. \end{split}$$

(Note that  $\mathfrak{A}\models t=s\iff \forall x,y\in |\mathfrak{A}|.\ \mathfrak{A}[x,y]\models t=s.$ )

B. KA terms w.r.t. binary relations and word languages

For a set X, we write  $X^*$  for the set of all finite sequences (i.e., words) over X. We write I for the empty word. We write wv for the concatenation of words w and v. For set  $L, K \subseteq$  $\Sigma^*$ , the *composition*  $L \cdot K$  is defined by:

$$L \cdot K \triangleq \{wv \mid w \in L \land v \in K\}.$$

The (word) language  $[t] \subseteq \Sigma^*$  of a KA term t is defined by:

$$[a] \triangleq \{a\}$$

$$[\bot] \triangleq \emptyset$$

$$[t \cup s] \triangleq [t] \cup [s]$$

$$[I] \triangleq \{I\}$$

$$[t \cdot s] \triangleq [t] \cdot [s]$$

$$[t^*] \triangleq \bigcup_{n \in \mathbb{N}} [t^n].$$

Interestingly, for KA terms, it is well-known that the equational theory w.r.t. binary relations coincides with that under the (single) word language interpretation (see, e.g., [6, Thm. 4]): for every KA terms t, s, we have

$$\models_{\text{REL}} t \leq s \iff [t] \subseteq [s].$$
 (†)

 $^6a^G$  is redundant for each  $a\in \Sigma_1^{(-)}\setminus \Sigma$  because it is determined by the other relations. However, this definition is compatible with the later.

The following follows from (†) and the known results in regular expressions [18, p. 3] ([19], for precise constructions):

**Proposition 3** ([19, Thm. 2.7], [18]). *The equational theory of*  $\mathcal{T}_{\{\cdot,\cup\}}$  (w.r.t. binary relations) is coNP-complete.

**Proposition 4** ([19, Prop. 2.4], [18]). The equational theory of  $\mathcal{T}_{\{\cdot,\cup,\_^*\}}$  (w.r.t. binary relations) is PSPACE-complete.

They can show the lower bounds of Thms. 24, 41, 44.

Remark 5. The equivalence (†) breaks if we add  $\cap$ ,  $\_$ , or  $\top$  by a standard word language interpretation [6, Sect. 4]. Note that (†) also breaks if we add  $a^-$  or  $I^-$  with  $[a^-] \triangleq \Sigma^* \setminus \{a\}$  and  $[I^-] \triangleq \Sigma^* \setminus \{I\}$ , respectively. For example,  $\models_{\text{REL}} \Box a \Box b \Box = \Box b \Box a \Box b$  holds [6, p. 13], but their languages are not the same. Here,  $\Box$  abbreviates the term  $c \cup \overline{c}$  (cf. Equation (1)) where c is any. Conversely, for example,  $[a^-] = [I \cup (\Sigma \setminus \{a\}) \cup (\Sigma \cdot \Sigma \cdot \Sigma^*)]$  holds, but such an equation does not hold in relational semantics (where a finite set  $L = \{t_1, \ldots, t_n\}$  of terms abbreviates the term  $t_1 \cup \cdots \cup t_n$ , here).

## C. PCoR\* and graph languages

Recall Sect. II-A. Using graph languages rather than word languages, we can give a characterization of the equational theory w.r.t. binary relations for more general terms (e.g., [6]). We use the following three operations on graphs, *series-composition*  $(\cdot)$ , *parallel-composition*  $(\cap)$ , and *converse*  $(\_)$ :

$$G \cdot H \triangleq \bullet \bigcirc -G \rightarrow \bigcirc -H \rightarrow \bigcirc \bullet \qquad G \cap H \triangleq \bullet \bigcirc \stackrel{G}{\longrightarrow} \bigcirc \bullet \rightarrow \bigcirc G \rightarrow \bigcirc \bullet \qquad G \cap H \triangleq \bullet \bigcirc G \rightarrow \bigcirc \bullet \rightarrow \bigcirc G \rightarrow \bigcirc G \rightarrow \bigcirc \bullet \rightarrow \bigcirc G \rightarrow \bigcirc G$$

The following is inspired by [8], [6, Def. 15] for PCoR\*, where we extend the definition of  $a^-$  and  $I^-$  for ECoR\*.

**Definition 6** (cf. [8], [6, Def. 15]). The graph language  $\mathcal{G}(t)$  of an ECoR\* term t is a set of graphs over  $\Sigma_{L}^{(-)}$ , defined by:

**Definition 7.** For a graph G over  $\Sigma_1^{(-)}$ , the *binary relation*  $[\![G]\!]_{\mathfrak{A}}\subseteq |\mathfrak{A}|^2$  on a structure  $\mathfrak{A}$  is defined by:

$$\langle x, y \rangle \in \llbracket G \rrbracket_{\mathfrak{A}} \quad \iff \quad (G \longrightarrow \mathfrak{A}[x, y]).$$

 $(G \longrightarrow H \text{ denotes that there is a homomorphism from } G \text{ to } H.)$  For each graph language  $\mathcal{G}$ , let

$$[\![\mathcal{G}]\!]_{\mathfrak{A}} \triangleq \bigcup_{G \in \mathcal{G}} [\![G]\!]_{\mathfrak{A}}.$$

Based on  $[\![G]\!]_{\mathfrak{A}}$  and  $[\![G]\!]_{\mathfrak{A}}$ , we use  $\models$  (Notation 2) also for graphs and graph languages. Note that:

$$\ddot{\mathfrak{A}} \models G \iff G \longrightarrow \ddot{\mathfrak{A}}; \quad \ddot{\mathfrak{A}} \models \mathcal{G} \iff \exists G \in \mathcal{G}.G \longrightarrow \ddot{\mathfrak{A}}.$$

The graph languages above characterize the relational semantics and the equational theory for PCoR\*, as follows (Prop. 8 is shown by induction on t and Prop. 9 is shown by using Prop. 8; see Appendix C, for more details):

**Proposition 8.** For every structure  $\mathfrak{A}$  and  $PCoR^*$  term t,

$$[t]_{\mathfrak{A}} = [\mathcal{G}(t)]_{\mathfrak{A}}.$$

**Proposition 9** ([8, Thm. 3.9], [6, Thm. 16]). For every PCoR\* terms t, s, we have

$$\models_{\text{REL}} t \leq s \iff \forall G \in \mathcal{G}(t).\exists H \in \mathcal{G}(s). \ H \longrightarrow G.$$

$$\mathcal{G}(a\cap b) = \{ + \bigcirc a \Rightarrow b \}; \mathcal{G}(a\cap (\top b)) = \{ + \bigcirc a \Rightarrow b \}.$$

## IV. GRAPH CHARACTERIZATION FOR ECOR\*

We consider extending Props. 8, 9 for ECoR\*. We can straightforwardly extend Prop. 8.

**Proposition 11** (cf. Prop. 8). For every structure  $\mathfrak{A}$  and ECoR\* term t, we have  $[\![t]\!]_{\mathfrak{A}} = [\![\mathcal{G}(t)]\!]_{\mathfrak{A}}$ .

*Proof.* Similar to Prop. 8 (Appendix D). 
$$\Box$$

However, we cannot extend Prop. 9, immediately.

Example 12.  $\models_{\text{REL}} \top \leq a \cup \overline{a}$  holds (cf. Equation (1)), but the right-hand side formula of Prop. 9 fails because there does not exist any homomorphism from any graphs in  $\mathcal{G}(a \cup \overline{a})$ :

$$\mathcal{G}(a \cup \overline{a}) = \left\{ \begin{array}{ccc} \bullet \bigcirc & a \to \bigcirc \bullet & , & \bullet \bigcirc & \overline{a} \to \bigcirc \bullet \end{array} \right\}$$
 
$$\mathcal{G}(\top) \ni \qquad \bullet \bigcirc \qquad \bigcirc \bullet \quad .$$

(The same problem occurs even without  $\top$ ; consider  $\models_{\text{REL}} b \cup \overline{b} \leq a \cup \overline{a}$  where  $b \neq a$ .)

To avoid the problem above, we consider modifying the graph languages using *edge saturations*.

# A. Edge-saturated graphs and 2-pointed structures

For a binary relation R, we write  $R^{\mathcal{E}}$  for the *equivalence* closure of R (the minimal equivalence relation subsuming R).

For a graph G over  $\Sigma_{\mathbf{I}}^{(-)}$ , we write  $G^{\mathcal{Q}}$  for the quotient graph G of G w.r.t. the equivalence relation  $(|G|^{\mathcal{E}})^{\mathcal{E}}$ ; e.g., if  $G = \underbrace{\bullet 0}_{\mathbf{I} - 2 - b} \underbrace{\bullet 0}_{\mathbf{I}$ 

**Definition 13.** Let G be a graph over  $\Sigma_1^{(-)}$ . We say that G is *consistent* if for every  $a \in \Sigma_1$ , the following holds:

(a-consistent)  $((\mathsf{I}^G)^{\mathcal{E}} \cdot a^G \cdot (\mathsf{I}^G)^{\mathcal{E}}) \cap ((\mathsf{I}^G)^{\mathcal{E}} \cdot \overline{a}^G \cdot (\mathsf{I}^G)^{\mathcal{E}}) = \emptyset$ . We say that G is (consistently) edge-saturated if G is consistent and the following hold:

(a-saturated) 
$$a^G \cup \overline{a}^G = |G|^2$$
, for every  $a \in \Sigma_1$ ;

<sup>7</sup>Precisely,  $G^{\mathcal{Q}}$  is the graph over  $\Sigma_{\mathbf{I}}^{(-)}$ , defined by  $|G^{\mathcal{Q}}| = \{[x]_G \mid x \in G\}$ ;  $a^{G^{\mathcal{Q}}} = \{\langle X, Y \rangle \in |G^{\mathcal{Q}}|^2 \mid \exists x \in X. \ \exists y \in Y. \ \langle x, y \rangle \in a^G\}$  for  $a \in \Sigma_{\mathbf{I}}^{(-)}$ ;  $\langle \mathbf{I}^{G^{\mathcal{Q}}}, \mathbf{2}^{G^{\mathcal{Q}}} \rangle = \langle [\mathbf{I}^G]_G, [\mathbf{2}^G]_G \rangle$ .

(I-equivalence)  $I^G$  is an equivalence relation.

Each edge-saturated graph induces a 2-pointed structure:

**Proposition 14.** If a graph G over  $\Sigma_{\mathsf{l}}^{(-)}$  is edge-saturated, then  $G^{\mathcal{Q}}$  is a 2-pointed structure.

*Proof.*  $I^{G^{\mathcal{Q}}}$  is the identity relation because  $I^{G}$  is an equivalence relation (I-equivalence). For  $a \in \Sigma_{\mathsf{I}}$ ,  $\bar{a}^{G^{\mathcal{Q}}} = |G^{\mathcal{Q}}|^2 \backslash a^{G^{\mathcal{Q}}}$  holds because  $a^{G^{\mathcal{Q}}} \cup \bar{a}^{G^{\mathcal{Q}}} = |G^{\mathcal{Q}}|^2$  (a-saturated) and  $a^{G^{\mathcal{Q}}} \cap \bar{a}^{G^{\mathcal{Q}}} = \emptyset$  (a-consistent). Thus,  $G^{\mathcal{Q}}$  is a 2-pointed structure.

# B. Graph characterization via edge saturations

**Definition 15.** For graphs G, H over  $\Sigma_1^{(-)}$ , we say that H is an *edge-extension* of G, if |H| = |G| and  $a^H \supseteq a^G$  for every  $a \in \Sigma_1^{(-)}$ . We say that H is an *(edge-)saturation* of G if H is an edge-extension of G and is edge-saturated.

Let S(G) be the set of all saturations of G.

For a graph language  $\mathcal{G}$ , let  $\mathcal{S}(\mathcal{G}) \triangleq \bigcup_{G \in \mathcal{G}} \mathcal{S}(G)$  and  $\mathcal{Q}(\mathcal{G}) \triangleq \{G^{\mathcal{Q}} \mid G \in \mathcal{G}\}$ . We abbreviate  $\mathcal{Q} \circ \mathcal{S}$  to  $\mathcal{Q}\mathcal{S}$ .

Example 16. When  $\Sigma = \{a\}$ ,  $QS(\rightarrow \circ \rightarrow )$  is the set:

 $\mathcal{QS}(\ \ \ \ \ \ \ \ )$  has 18 graphs up to isomorphism (the sum of patterns  $(2^{1\times 1}=2)$  when the two vertices are connected with I and patterns  $(2^{2\times 2}=16)$  otherwise). For every G in  $\mathcal{QS}(\ \ \ \ \ \ \ \ \ \ )$ , there exists a homomorphism to G from 0 or 0 or 0, as 0 is edge-saturated:

$$\mathcal{G}(a \cup \overline{a}) = \left\{ \begin{array}{c} \bullet \Diamond - \overline{a} \bullet \Diamond \bullet & , \quad \bullet \Diamond - a \bullet \Diamond \bullet \end{array} \right\}$$
 
$$\mathcal{QS}(\mathcal{G}(\top)) = \left\{ \begin{array}{c} \bullet \Diamond \bullet & , \quad \bullet \Diamond \bullet \\ \stackrel{\bullet}{a} & \stackrel{\bullet}{a} & \stackrel{\bullet}{a} \end{array} \right. \begin{array}{c} \stackrel{\bullet}{a} & \stackrel{\bullet}{a} \\ \stackrel{\bullet}{a} & \stackrel{\bullet}{a} & \stackrel{\bullet}{a} \end{array} \right. , \dots \right\}$$

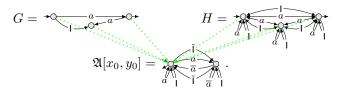
As above, by using  $QS(\mathcal{G}(\top))$  instead of  $\mathcal{G}(\top)$ , we can avoid the problem in Example 12. Using QS, we can strengthen Prop. 9 ([8, Thm. 3.9], [6, Thm. 16]), for ECoR\*, as Thm. 18. We first show the following:

**Lemma 17.** For any graph G over  $\Sigma_{\mathbf{l}}^{(-)}$ ,  $[\![G]\!]_{\mathfrak{A}} = [\![\mathcal{QS}(G)]\!]_{\mathfrak{A}}$ .

*Proof.* We prove that for any G, both  $[\![G]\!]_{\mathfrak{A}} = [\![S(G)]\!]_{\mathfrak{A}}$  and  $[\![G]\!]_{\mathfrak{A}} = [\![G^{\mathcal{Q}}]\!]_{\mathfrak{A}}$ , respectively.

For  $[\![G]\!]_{\mathfrak{A}} = [\![S(G)]\!]_{\mathfrak{A}}$ :  $(\supseteq)$ : If  $H \in S(G)$  and  $h: H \longrightarrow \mathfrak{A}[x_0,y_0]$ , then  $h: G \longrightarrow \mathfrak{A}[x_0,y_0]$  because H is a saturation of G.  $(\subseteq)$ : If  $h: G \longrightarrow \mathfrak{A}[x_0,y_0]$ , let H be the saturation of G s.t.  $a^H = \{\langle x,y \rangle \mid \langle h(x),h(y) \rangle \in a^{\mathfrak{A}} \}$  for  $a \in \Sigma_1^{(-)}$ . Then  $h: H \longrightarrow \mathfrak{A}[x_0,y_0]$ . Here, H is an edge-extension of G because  $\langle x,y \rangle \in a^G \Longrightarrow \langle h(x),h(y) \rangle \in a^{\mathfrak{A}} \Longrightarrow \langle x,y \rangle \in a^H$ ; H is edge-saturated because  $\mathfrak{A}$  is edge-saturated; thus, H is indeed a saturation of G. For example, from the homomorphism for  $G \longrightarrow \mathfrak{A}[x_0,y_0]$ , by filling non-existing edges in G

so that they map to edges of  $\mathfrak{A}$ , we can construct the saturation H of G s.t.  $H \longrightarrow \mathfrak{A}[x_0, y_0]$ , as follows:



For  $\llbracket G \rrbracket_{\mathfrak{A}} = \llbracket G^{\mathcal{Q}} \rrbracket_{\mathfrak{A}}$ :  $(\supseteq)$ : If  $G^{\mathcal{Q}} \longrightarrow \mathfrak{A}[x_0, y_0]$ , then  $G \longrightarrow \mathfrak{A}[x_0, y_0]$  because  $G \longrightarrow G^{\mathcal{Q}}$  by the quotient map (with transitivity of  $\longrightarrow$ ).  $(\subseteq)$ : If  $h \colon G \longrightarrow \mathfrak{A}[x_0, y_0]$ , then  $h \circ g \colon G^{\mathcal{Q}} \longrightarrow \mathfrak{A}[x_0, y_0]$ , where g is a section of the quotient map from G to  $G^{\mathcal{Q}}$  (a map g s.t.  $g(X) \in X$  for  $X \in |G^{\mathcal{Q}}|$ ). Hence,  $\llbracket G \rrbracket_{\mathfrak{A}} = \llbracket \mathcal{S}(G) \rrbracket_{\mathfrak{A}} = \llbracket \mathcal{Q}\mathcal{S}(G) \rrbracket_{\mathfrak{A}}$ .

**Theorem 18** (cf. Prop. 9). For every ECoR\* terms t, s,

$$\models_{\text{REL}} t \leq s \iff \forall G \in \mathcal{QS}(\mathcal{G}(t)).\exists H \in \mathcal{G}(s). \ H \longrightarrow G.$$

*Proof.* By the following formula transformation:

$$\models_{\text{REL}} t \leq s \iff \forall \mathfrak{A}. \ \llbracket t \rrbracket_{\mathfrak{A}} \subseteq \llbracket s \rrbracket_{\mathfrak{A}} \qquad \text{(Def. of } \models_{\text{REL}})$$

$$\iff \forall \mathfrak{A}. \ \llbracket \mathcal{QS}(\mathcal{G}(t)) \rrbracket_{\mathfrak{A}} \subseteq \llbracket \mathcal{G}(s) \rrbracket_{\mathfrak{A}} \qquad \text{(Prop. 11, Lem. 17)}$$

$$\iff \forall \mathfrak{A}. \forall G \in \mathcal{QS}(\mathcal{G}(t)). \ \llbracket G \rrbracket_{\mathfrak{A}} \subseteq \llbracket \mathcal{G}(s) \rrbracket_{\mathfrak{A}} \qquad \text{(Def. of } \llbracket \rrbracket)$$

$$\iff \forall G \in \mathcal{QS}(\mathcal{G}(t)). \forall \mathfrak{A}. \ \llbracket G \rrbracket_{\mathfrak{A}} \subseteq \llbracket \mathcal{G}(s) \rrbracket_{\mathfrak{A}}$$

$$\iff \forall G \in \mathcal{QS}(\mathcal{G}(t)). \forall \mathfrak{A}.$$

$$(G \longrightarrow \mathfrak{A}) \text{ implies } (\exists H \in \mathcal{G}(s). \ H \longrightarrow \mathfrak{A}) \text{ (Def. of } \llbracket \rrbracket)$$

$$\iff \forall G \in \mathcal{QS}(\mathcal{G}(t)). \exists H \in \mathcal{G}(s). \ H \longrightarrow G. \qquad (\heartsuit)$$

Here, for  $(\heartsuit)$ ,  $\iff$ : Let  $H \in \mathcal{G}(s)$  be such that  $H \longrightarrow G$ . Then for any 2-pointed structure  $\ddot{\mathfrak{A}}$  s.t.  $G \longrightarrow \ddot{\mathfrak{A}}$ , we have  $H \longrightarrow \ddot{\mathfrak{A}}$  by transitivity of  $\longrightarrow$ .  $\Longrightarrow$ : By letting  $\ddot{\mathfrak{A}} = G$ . Note that G is a 2-pointed structure since  $G \in \mathcal{QS}(\mathcal{G}(t))$  (Prop. 14).

## C. Bounded model property

Thm. 18 gives an upper bound for the equational theories of existential calculi of relations. Note that the model checking problem of ECoR\* is decidable in polynomial time.

**Proposition 20.** The following problem is decidable in  $\mathcal{O}(\|t\| \times \#(|\ddot{\mathfrak{A}}|)^{\omega})$  time: given a finite 2-pointed structure  $\ddot{\mathfrak{A}}$  and an ECoR\* term t, does  $\ddot{\mathfrak{A}} \models t$  hold? Here,  $\omega$  is the matrix multiplication exponent.

Proof Sketch. Let  $\ddot{\mathfrak{A}} = \mathfrak{A}[x,y]$ . For  $s \in \operatorname{Sub}(t)$ , let  $f_s \colon |\mathfrak{A}| \times |\mathfrak{A}| \to \{\operatorname{true}, \operatorname{false}\}$  be such that  $f_s(x,y) = \operatorname{true}$  iff  $\langle x,y \rangle \in [\![s]\!]_{\mathfrak{A}}$ . Here,  $\operatorname{Sub}(t)$  denotes the set of all sub-terms of t. Then the function tables of  $\{f_s\}_{s \in \operatorname{Sub}(t)}$  can be calculated by a simple dynamic programming on s, where for the case  $s = u^*$ , we use the algorithm for the transitive closure of boolean matrix [31].

**Lemma 21** (bounded model property). For every ECoR\* terms t, s, we have:  $\not\models_{\text{REL}} t \leq s \iff$  there exists a 2-pointed structure  $\ddot{\mathfrak{A}} \in \mathcal{QS}(\mathcal{G}(t))$  such that  $\ddot{\mathfrak{A}} \not\models t \leq s$ .

Proof.  $\iff$ : Trivial.  $\implies$ : Let  $\ddot{\mathfrak{A}}=\mathfrak{A}[x,y]\in\mathcal{QS}(\mathcal{G}(t))$  be a 2-pointed structure such that  $\forall H\in\mathcal{G}(s), H\not\to\ddot{\mathfrak{A}}$  (Thm. 18). Then  $\langle x,y\rangle\in\llbracket\mathcal{QS}(\mathcal{G}(t))\rrbracket_{\mathfrak{A}}$  because  $\mathcal{QS}(\mathcal{G}(t))\ni\ddot{\mathfrak{A}}\to\mathfrak{A}[x,y]$  ( $\longrightarrow$  is reflexive).  $\langle x,y\rangle\not\in\llbracket\mathcal{G}(s)\rrbracket_{\mathfrak{A}}$  because  $\forall H\in\mathcal{G}(s). H\not\to\ddot{\mathfrak{A}}$  (Def. of  $\llbracket\rrbracket_{\mathfrak{A}}$ ). Thus  $\langle x,y\rangle\in\llbracket t\rrbracket_{\mathfrak{A}}$  and  $\langle x,y\rangle\not\in\llbracket s\rrbracket_{\mathfrak{A}}$  (Prop. 11, Lem. 17). Hence  $\ddot{\mathfrak{A}}\not\models t\leq s$ .

# **Lemma 22.** The equational theory of ECoR\* is in $\Pi_1^0$ .

*Proof.* Since  $\not\models_{\text{REL}} t = s$  if and only if  $(\not\models_{\text{REL}} t \leq s) \lor (\not\models_{\text{REL}} s \leq t)$ , it suffices to show that the following problem is in  $\Sigma^0_1$ : given ECoR\* terms t, s, does  $\not\models_{\text{REL}} t \leq s$  hold? This follows from Lem. 21 with Prop. 20. Note that for every  $G \in \mathcal{QS}(\mathcal{G}(t))$ , #(|G|) is always finite, and that we can easily enumerate the graphs in  $\mathcal{QS}(\mathcal{G}(t))$ .

Particularly for ECoR (not ECoR\*), graphs of each term t have a linear number of vertices in the size ||t||.

**Proposition 23.** For every ECoR term t and  $G \in \mathcal{QS}(\mathcal{G}(t))$ , we have  $\#(|G|) \leq 1 + \|t\|$ .

*Proof Sketch.* By easy induction on t, we have: for every  $H \in \mathcal{G}(t)$ ,  $\#(|H|) \le 1 + \|t\|$ . Also  $\#(|G|) \le \#(|H|)$  is clear for every  $G \in \mathcal{QS}(H)$ .

**Theorem 24.** The equational theory of ECoR is coNP-complete.

*Proof.* For hardness: By Prop. 3, as ECoR subsumes  $\mathcal{T}_{\{\cdot,\cup\}}$ . For upper bound: Similarly for Lem. 22, we show that the following problem is in NP: given ECoR terms t,s, does  $\not\models_{\text{REL}} t \leq s$  hold? By Lem. 21, we can give the following algorithm:

- 1) Take a graph  $H \in \mathcal{G}(t)$  non-deterministically according to the definition of  $\mathcal{G}$ ; then take a graph  $G \in \mathcal{S}(H)$ , non-deterministically (G is a graph in  $\mathcal{S}(\mathcal{G}(t))$ ).
- 2) Return true if  $G^{\mathcal{Q}} \not\models t \leq s$ ; false otherwise.

Then  $\not\models_{\text{REL}} t \leq s$  if some execution returns true;  $\models_{\text{REL}} t \leq s$  otherwise. Here,  $G^{\mathcal{Q}} \not\models t \leq s$  can be decided in polynomial time by Prop. 20 with  $\#(|G^{\mathcal{Q}}|) \leq 1 + \|t\|$  (Prop. 23).

# V. SATURABLE PATHS: SATURATIONS FROM A PATH GRAPH FOR INTERSECTION-FREE FRAGMENTS

In this section, we refine the graph characterization of edgesaturations (in the previous section) for ECoR\* without intersection (ExKA, for short; Sect. III-A) by using *saturable paths*. Using this characterization, we can show the decidability of the equational theory (Thm. 33) and give an automata construction for two smaller fragments (Thms. 40, 43).

## A. NFAs as terms

A non-deterministic finite automaton with epsilon translations I (NFA, for short)  $\mathcal{A} = \langle |\mathcal{A}|, \{a^{\mathcal{A}}\}_{a \in A}, 1^{\mathcal{A}}, 2^{\mathcal{A}} \rangle$  over a set A (with A containing a designated element I) is a graph

over A. The transition relation  $\delta_w^{\mathcal{A}}$  of a word  $w = a_1 \dots a_n \in (A \setminus \{1\})^*$  is defined by:

$$\delta_w^{\mathcal{A}} \triangleq (\mathsf{I}^{\mathcal{A}})^* \cdot a_1^{\mathcal{A}} \cdot (\mathsf{I}^{\mathcal{A}})^* \cdot \ldots \cdot (\mathsf{I}^{\mathcal{A}})^* \cdot a_n^{\mathcal{A}} \cdot (\mathsf{I}^{\mathcal{A}})^*.$$

For notational simplicity, for  $x \in |\mathcal{A}|$  and  $X \subseteq |\mathcal{A}|$ , let  $\delta_w^{\mathcal{A}}(x) \triangleq \{y \mid \langle x,y \rangle \in \delta_w^{\mathcal{A}}\}$  and  $\delta_w^{\mathcal{A}}(X) \triangleq \bigcup_{x \in X} \delta_w^{\mathcal{A}}(x)$ . The language  $[\mathcal{A}]$  of  $\mathcal{A}$  is defined by:

$$[\mathcal{A}] \triangleq \{ w \in (A \setminus \{\mathsf{I}\})^* \mid 2^{\mathcal{A}} \in \delta_w^{\mathcal{A}}(1^{\mathcal{A}}) \}.$$

Let  $\Sigma_{\mathbf{I}}^{(-,\smile)} \triangleq \{a,a^\smile \mid a \in \Sigma^{(-)}\} \cup \{\mathbf{I},\mathbf{I}^-\}$ . Similarly for  $\bar{t}$ , for each  $t \in \Sigma_{\mathbf{I}}^{(-,\smile)} \cup \{\bot,\top\}$ ,  $\check{t}$  denotes the following term, where  $a \in \Sigma^{(-)}$ :

$$\widecheck{a} \triangleq a^{\smile} \quad \widecheck{a^{\smile}} \triangleq a \quad \widecheck{\mathbf{I}} \triangleq \mathbf{I} \quad \widecheck{\mathbf{I}}^{-} \triangleq \mathbf{I}^{-} \quad \widecheck{\mathbf{T}} \triangleq \mathbf{T} \quad \widecheck{\bot} \triangleq \bot.$$

In the following, we always consider NFAs over the set  $\Sigma_{1}^{(-,\smile)}$  (where I is used as epsilon transitions).

For an NFA  $\mathcal{A}$  over  $\Sigma_{\mathsf{I}}^{(-,\smile)}$ , the *binary relation*  $[\![\mathcal{A}]\!]_{\mathfrak{A}} \subseteq |\mathcal{A}|^2$  is defined by:

$$[\![\mathcal{A}]\!]_{\mathfrak{A}} \triangleq \bigcup_{w \in [\mathcal{A}]} [\![w]\!]_{\mathfrak{A}}.$$

Naturally, we can give a construction from ExKA terms to NFAs using Thompson's construction [32], as follows:

**Definition 25.** The NFA  $A_t$  of an ExKA term t is defined by:

$$\mathcal{A}_{a} \triangleq \bullet \bigcirc -a \rightarrow \bigcirc \bullet \quad (a \in \Sigma_{1}^{(-, \smile)} \setminus \{I\}) \quad \mathcal{A}_{1} \triangleq \bullet \bigcirc -1 \rightarrow \bigcirc \bullet$$

$$\mathcal{A}_{t \cup s} \triangleq \bullet \bigcirc -A_{t} \rightarrow \bigcirc -1 \rightarrow \bigcirc \bullet \quad \mathcal{A}_{1} \triangleq \bullet \bigcirc \bullet$$

$$\mathcal{A}_{t \cdot s} \triangleq \bullet \bigcirc -A_{t} \rightarrow \bigcirc -1 \rightarrow \bigcirc -A_{s} \rightarrow \bigcirc \bullet \quad \mathcal{A}_{T} \triangleq \mathcal{A}_{a \cup \overline{a}}$$

$$\mathcal{A}_{t^{*}} \triangleq \bullet \bigcirc -A_{t} \rightarrow \bigcirc -1 \rightarrow \bigcirc -A_{t} \rightarrow \bigcirc \bullet \quad .$$

**Proposition 26.** For every structure  $\mathfrak{A}$  and ExKA term t, we have  $[\![t]\!]_{\mathfrak{A}} = [\![A_t]\!]_{\mathfrak{A}}$ .

Proof Sketch. Let s be the term t in which each  $\top$  has been replaced with  $a \cup \overline{a}$ . Then,  $[\![s]\!]_{\mathfrak{A}} = [\![t]\!]_{\mathfrak{A}}$  holds by Equation (1) and  $\mathcal{A}_s$  coincides with  $\mathcal{A}_t$  (by Def. 25). By viewing s as the regular expression over  $\Sigma_1^{(-,\smile)} \setminus \{1\}$ , we have  $[s] = [\mathcal{A}_s]$  [32]. By straightforward induction on s using the distributivity,  $[\![s]\!]_{\mathfrak{A}} = \bigcup_{w \in [s]} [\![w]\!]_{\mathfrak{A}}$  (Appendix E). Thus  $[\![t]\!]_{\mathfrak{A}} = [\![s]\!]_{\mathfrak{A}} = \bigcup_{w \in [\mathcal{A}_s]} [\![w]\!]_{\mathfrak{A}} = [\![\mathcal{A}_s]\!]_{\mathfrak{A}} = [\![\mathcal{A}_t]\!]_{\mathfrak{A}}$ .

Thanks to the above proposition, we work directly with NFAs rather than terms in the sequel.

#### B. Saturable paths

For a word  $w \in (\Sigma_1^{(-, \smile)} \setminus \{1\})^*$ , we use G(w) to denote the unique graph in  $\mathcal{G}(w)$  (Def. 6), up to isomorphism. Here, each vertex in G(w) is indexed by a number in [0, n], from the left to the right, where  $w = a_1 \dots a_n$ . For example,

$$G(\bar{l}a \bar{a}) = +0 - \bar{l} + 0 - \bar{a} = 0$$
.

For each w, G(w) is a path graph (by forgetting labels and directions of edges).

Recall  $[\![A]\!]_{\mathfrak{A}}$  in Sect. V-A. Based on  $[\![A]\!]_{\mathfrak{A}}$ , we use  $\models$  (Notation 2) also for automata. Note that:

$$\ddot{\mathfrak{A}} \models \mathcal{A} \iff \exists w \in [\mathcal{A}]. \ \ddot{\mathfrak{A}} \models w \qquad \text{(Def. of } \llbracket \mathcal{A} \rrbracket_{\mathfrak{A}})$$
$$\iff \exists w \in [\mathcal{A}]. \ G(w) \longrightarrow \ddot{\mathfrak{A}}. \qquad \text{(Prop. 11)}$$

In this subsection, we consider the following saturability problem: given an NFA  $\mathcal{A}$  and a word w, is there a saturation H of G(w) such that  $H^{\mathcal{Q}} \not\models \mathcal{A}$ ? (Recall  $H^{\mathcal{Q}}$  (Prop. 14).) This problem can apply to the equational theory (Thm. 33). For this problem, we introduce *saturable paths*.

*Example* 27. Let  $\Sigma = \{a\}$ . Let  $\mathcal{A}$  be the NFA obtained from the term  $\overline{a} \cdot \overline{a} \cdot \overline{a}^*$  and  $w = \overline{a}$ :

$$\mathcal{A} = \bullet \widehat{\mathbb{A}} - \overline{a} - \widehat{\mathbb{B}} - \overline{a} - \widehat{\mathbb{C}} \bullet \qquad G(w) = \bullet \widehat{\mathbb{O}} - \overline{a} - \widehat{\mathbb{O}} \bullet \qquad .$$

Let us consider constructing a saturation H of G(w) such that  $H^{\mathcal{Q}} \not\models \mathcal{A}$ . In this case, the following  $H_1$  is the unique solution  $(H_2, H_3, H_4)$  are not the solution because  $C \in U_1$ :

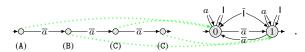
$$H_1 = \begin{array}{c} a & \overline{a} & \overline{a} \\ \hline 0 & \overline{a} & 1 \\ \hline (A) & (B) \end{array} \qquad \begin{array}{c} H_2 = \begin{array}{c} a & \overline{a} & \overline{a} \\ \hline 0 & \overline{a} & 1 \\ \hline (A,C) & (B,C) \\ \hline \end{array}$$

$$H_3 = \begin{array}{c} \overline{a} & \overline{a} & \overline{a} \\ \hline (A,B,C) & (B,C) \\ \hline \end{array} \qquad \begin{array}{c} H_4 = \begin{array}{c} a & \overline{a} & \overline{a} \\ \hline 0 & \overline{a} & \overline{a} \\ \hline \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \hline \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{a} \end{array} \qquad \begin{array}{c} \overline{a} & \overline{a} \\ \overline{a} & \overline{$$

Here the states under each vertex denote that they are reachable from the state A on the vertex 0; more precisely, each set  $U_i \subseteq |\mathcal{A}|$  (where  $i \in |G(w)|$ ) is defined by:

$$z \in U_i \iff \exists v \in [\mathcal{A}[\_, z]]. \ G(v) \longrightarrow H^{\mathcal{Q}}[\_, [i]_H].$$

Here,  $\mathcal{A}[\_,z]$  denotes the graph  $\mathcal{A}$  in which  $2^{\mathcal{A}}$  has been replaced with z (similarly for  $H^{\mathcal{Q}}[\_,[i]_H]$ ). By definition,  $H^{\mathcal{Q}}\not\models\mathcal{A}$  (iff  $\neg(\exists v\in[\mathcal{A}].\ G(v)\longrightarrow H^{\mathcal{Q}})$ ) iff  $2^{\mathcal{A}}\not\in U_{2^H}$ . For example, in  $H_2$ ,  $\mathbf{C}\in U_1$  because  $G(\overline{a}\ \overline{a}\ \overline{a})\longrightarrow H_2^{\mathcal{Q}}$  holds by:



In contrast, in  $H_1$ , because  $C \notin U_1$  (i.e.,  $\forall v \in [A]$ .  $G(v) \not\longrightarrow H_1^{\mathcal{Q}}$ ) holds, we have  $H_1^{\mathcal{Q}} \not\models A$ .

Consider the following P, which is the graph G(w) with an equivalence relation I, its complement  $\bar{I}$ , and  $\{U_i\}_{i\in |G(w)|}$ :

$$P = \begin{array}{c} \downarrow \\ \downarrow \\ 0 \\ \hline a \\ \downarrow \\ 0 \\ \hline a \\ B \\ \end{array}.$$

Using only the data of P, we can show the existence of a saturation of G(w). For each pair  $\langle i,j \rangle$  of vertices, if  $(\delta_a^{\mathcal{A}}(U_i) \subseteq U_j \text{ and } \delta_{\tilde{a}}^{\mathcal{A}}(U_j) \subseteq U_i)$  or  $(\delta_{\overline{a}}^{\mathcal{A}}(U_i) \subseteq U_j \text{ and } \delta_{\tilde{a}}^{\mathcal{A}}(U_j) \subseteq U_i)$  holds (cf. (P-Sat) in Def. 29), then we add either the a- or  $\overline{a}$ -labeled edge, according to this condition; for example, for the pair  $\langle 1,0 \rangle$ , since  $\delta_a^{\mathcal{A}}(U_1) = \emptyset \subseteq U_0$  and  $\delta_{\tilde{a}}^{\mathcal{A}}(U_0) = \emptyset \subseteq U_1$  hold, we add the edge for

 $\langle 1,0 \rangle \in a^H$  (we cannot add the edge for  $\langle 1,0 \rangle \in \overline{a}^H$  because  $\delta_{\overline{a}}^{\mathcal{A}}(U_1) = \{\mathtt{C}\} \not\subseteq U_0$ ). Note that  $\{U_i\}_{x \in |G(w)|}$  is invariant when we add edges in this strategy. By adding such edges as much as possible, we can give a saturation of G(w) from P preserving  $\{U_i\}_{x \in |G(w)|}$  (cf. Lem. 30); finally,  $H_1$  is obtained, as follows (from the left to the right):

$$(A) \qquad (B) \qquad (A) \qquad (B) \qquad (B)$$

Example 28 (another example with  $\_$  and  $\bar{I}$ ). Let  $\Sigma = \{a\}$ . Let A be the NFA obtained from  $\bar{I} \cdot (\check{a} \cdot \check{a})^*$  and  $w = a\bar{a}$ :

$$\mathcal{A} = \text{ for } G(w) = \text{ fo$$

Let us consider constructing a saturation H of G(w) such that  $H^{\mathcal{Q}} \not\models \mathcal{A}$ . Then, the following H is a solution (note that  $\mathcal{D} \not\in U_2$ ; thus,  $H^{\mathcal{Q}} \not\models \mathcal{A}$ ) and the following P is the corresponding saturable path:

$$H = \underbrace{0 \quad \overline{a} \quad \overline{a} \quad \overline{a} \quad \overline{a} \quad \overline{a}}_{(A, C) \quad (B, D) \quad (A, C)} P = \underbrace{0 \quad \overline{a} \quad \overline{a} \quad \overline{a} \quad 2}_{(A, C) \quad B, D} \quad A, C$$

(See Remark 45 for an example when there is no saturation.) Inspired by  $\{U_i\}_{i\in |G(w)|}$  above, for characterizing the saturability problem, we define *saturable paths*; they are path graphs with additional data (an equivalence relation I, its complement  $\bar{\mathbf{I}}$ , and  $\{U_i\}_{i\in |G(w)|}$ ) for taking saturations appropriately. For graphs G,H over  $\Sigma_1^{(-)}$ , we say that H is an I-saturation of G if H is an edge-extension of G such that

- for every  $a \in \Sigma^{(-)}$ ,  $a^H = a^G$ ;
- $I^H$  is an equivalence relation and  $\overline{I}^H = |H|^2 \setminus I^H$ ;
- *H* is consistent.

(By definition, H is uniquely determined from  $I^H$ , if exists.)

**Definition 29** (saturable path). For an NFA  $\mathcal A$  over  $\Sigma_{\mathsf{I}}^{(-,\smile)}$  and a word w over  $\Sigma_{\mathsf{I}}^{(-,\smile)}\setminus\{\mathsf{I}\}$ , consider a pair  $P=\langle G,\{U_i\}_{i\in |G|}\rangle$  of

- G an I-saturation of G(w);
- $U_i \subseteq |\mathcal{A}|$  for each  $i \in |G|$ .

For  $a \in \Sigma_{\mathbf{I}}^{(-,\smile)}$ , let

$$\operatorname{Con}_a^{\mathcal{A}}(U,U') \triangleq (\delta_a^{\mathcal{A}}(U) \subseteq U' \wedge \delta_{\check{a}}^{\mathcal{A}}(U') \subseteq U).$$

Then we say that P is a saturable path for  $\not\models_{REL} w \leq \mathcal{A}$  if the following three hold:

(P-s-t) 
$$1^{\mathcal{A}} \in U_{1^G}$$
 and  $2^{\mathcal{A}} \notin U_{2^G}$ ;  
(P-Con) for all  $a \in \Sigma_1^{(-)}$  and  $\langle i,j \rangle \in a^G$ ,  $\operatorname{Con}_a^{\mathcal{A}}(U_i,U_j)$ ;  
(P-Sat) for all  $a \in \Sigma_1$  and  $\langle i,j \rangle \in |G|^2$ ,  
 $\operatorname{Con}_a^{\mathcal{A}}(U_i,U_j) \vee \operatorname{Con}_{\overline{a}}^{\mathcal{A}}(U_i,U_j)$ .

Saturable paths can characterize the saturability problem, as Lem. 32. We first show the following:

**Lemma 30.** For every saturable path  $P = \langle G, \{U_i\}_{i \in |G|} \rangle$  for  $\not\models_{\text{REL}} w \leq \mathcal{A}$ , there is a saturation H of G such that **(P-Con')** for all  $a \in \Sigma_1^{(-)}$  and  $\langle i, j \rangle \in a^H$ ,  $\text{Con}_a^A(U_i, U_j)$ .

*Proof.* Starting from H = G, we add edges labeled with  $a \in \Sigma^{(-)}$  while preserving (P-Con'), by repeating the following:

• If  $\langle i,j \rangle \in (\mathsf{I}^H \cdot a^H \cdot \mathsf{I}^H) \setminus a^H$  for some  $a \in \Sigma^{(-)}$  and  $i,j \in |H|$ , we add the edge to H. Then,  $\mathrm{Con}_a^{\mathcal{A}}(U_i,U_j)$  holds as follows. Let i',j' be s.t.  $\langle i,i' \rangle \in \mathsf{I}^H, \langle i',j' \rangle \in a^H$ , and  $\langle j',j \rangle \in \mathsf{I}^H$ . For every  $z \in |\mathcal{A}|$ , we have

$$z \in U_{i'} \Longrightarrow z \in \delta_{\mathsf{I}}^{\mathcal{A}}(U_i)$$
  $(U_{i'} \subseteq \delta_{\mathsf{I}}^{\mathcal{A}}(U_i) \text{ (P-Con')})$   
 $\Longrightarrow z \in U_i$   $(\delta_{\mathsf{I}}^{\mathcal{A}} = (\mathsf{I}^{\mathcal{A}})^* \text{ is reflexive})$   
 $\cdots \Longrightarrow z \in U_{i'}.$   $(\mathsf{I}^H \text{ is symmetric})$ 

Thus  $U_i = U_{i'}$ . In the same way,  $U_j = U_{j'}$ . Hence  $\operatorname{Con}_a^{\mathcal{A}}(U_i, U_j)$  is derived from  $\operatorname{Con}_a^{\mathcal{A}}(U_{i'}, U_{j'})$ .

• Otherwise, since H is not edge-saturated,  $\langle i,j\rangle \not\in a^H \cup \overline{a}^H$  for some  $a \in \Sigma$  and  $i,j \in |H|$ . If  $\operatorname{Con}_a^{\mathcal{A}}(U_i,U_j)$  holds, then we add the edge for  $\langle i,j\rangle \in a^H$  to H. Otherwise, since  $\operatorname{Con}_{\overline{a}}^{\mathcal{A}}(U_i,U_j)$  holds by (P-Sat), we add the edge for  $\langle i,j\rangle \in \overline{a}^H$  to H.

Then H is a saturation of G, as follows. For (I-equivalence): Because G is an I-saturation. For (a-saturated): Clear. For (a-consistent): By that G is consistent and  $(\mathsf{I}^H \cdot a^H \cdot \mathsf{I}^H) \cap (\mathsf{I}^H \cdot \overline{a}^H \cdot \mathsf{I}^H) = \emptyset$  is preserved (by the construction of H).  $\square$ 

*Example* 31 (of Lem. 30). Recall A, w, and the saturable path  $P = \langle G, \{U_i\}_{i \in |G|} \rangle$  in Example 28.

$$G = \bullet 0 \qquad a \rightarrow 1 \qquad \overline{a} \rightarrow 2 \qquad G' = \bullet 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 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\overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 1 \qquad \overline{a} \rightarrow 2 \rightarrow 0 \qquad \overline{a} \rightarrow 2 \rightarrow 0$$

First, we add the a-labeled edge for  $\langle 2,1 \rangle$  because  $\langle 2,1 \rangle \in (\mathsf{I}^G \cdot a^G \cdot \mathsf{I}^G)$ ; similarly, we add the  $\overline{a}$ -labeled edge for  $\langle 1,0 \rangle$  (let G' be the graph). Second, we consider adding an a- or  $\overline{a}$ -labeled edge for  $\langle 0,2 \rangle$ . Then, because  $\mathrm{Con}_a^\mathcal{A}(\{\mathtt{A},\mathtt{C}\},\{\mathtt{A},\mathtt{C}\})$ , we add an a-labeled edge for  $\langle 0,2 \rangle$  (note that  $\neg \mathrm{Con}_{\overline{a}}^\mathcal{A}(\{\mathtt{A},\mathtt{C}\},\{\mathtt{A},\mathtt{C}\})$  because  $\delta_{\overline{a}}^\mathcal{A}(\{\mathtt{A},\mathtt{C}\}) = \{\mathtt{D}\} \not\subseteq \{\mathtt{A},\mathtt{C}\}$ ); we also add an a-labeled edge for  $\langle 2,0 \rangle$  because  $\langle 2,0 \rangle, \langle 0,2 \rangle \in \mathsf{I}^{G'}$  (let G'' be the graph). By adding the other edges similarly, the saturation H of G(w) can be obtained

**Lemma 32.** For an NFA  $\mathcal{A}$  over  $\Sigma_{1}^{(-,\smile)}$  and a word w over  $\Sigma_{1}^{(-,\smile)}\setminus\{1\}$ , the following are equivalent:

- There is a saturation H of G(w) such that  $H^{\mathcal{Q}} \not\models w \leq \mathcal{A}$ .
- There is a saturable path P for  $\not\models_{REL} w \leq A$ .

Proof.  $\Leftarrow$ : Let  $P = \langle G, \{U_i\}_{i \in |G|} \rangle$ . Let H be the saturation of G (Lem. 30). Then  $H^{\mathcal{Q}} \not\models w \leq \mathcal{A}$  holds as follows. For  $H^{\mathcal{Q}} \models w$ : Because  $G(w) \longrightarrow H \longrightarrow H^{\mathcal{Q}}$  (cf. Lem. 17). For  $H^{\mathcal{Q}} \not\models \mathcal{A}$ : Assume that  $H^{\mathcal{Q}} \models \mathcal{A}$ . Then there is a word  $a_1 \dots a_m \in [\mathcal{A}]$  such that  $G(a_1 \dots a_m) \longrightarrow H^{\mathcal{Q}}$ . By  $a_1 \dots a_m \in [\mathcal{A}]$ , there are  $z_0, \dots, z_m \in |\mathcal{A}|$  such that  $\langle z_0, z_m \rangle = \langle 1^{\mathcal{A}}, 2^{\mathcal{A}} \rangle$  and for  $k \in [m], z_k \in \delta_{a_k}^{\mathcal{A}}(z_{k-1})$ . By

 $G(a_1 \dots a_m) \longrightarrow H^{\mathcal{Q}}$ , there are  $l_0, \dots, l_m \in |H|$  such that  $\langle l_0, l_m \rangle = \langle 1^H, 2^H \rangle$  and for  $k \in [m], \langle l_{k-1}, l_k \rangle \in a_k^H$ . Then,

**Sublemma.** For every  $k \in [0, m]$ ,  $z_k \in U_{l_k}$ .

*Proof.* By induction on k. Case k=0: By  $1^{\mathcal{A}} \in U_{1^H}$  (P-s-t). Case k>1: We have

$$z_k \in \delta_{a_k}^{\mathcal{A}}(z_{k-1}) \subseteq \delta_{a_k}^{\mathcal{A}}(U_{l_{k-1}}) \qquad \text{(By } z_{k-1} \in U_{l_{k-1}} \text{ (IH))}$$
$$\subseteq U_{l_k}. \quad \text{(By } \langle l_{k-1}, l_k \rangle \in a_k^H \text{ (P-Con'))} \quad \Box$$

Since  $z_m \in U_{l_m}$  contradicts  $2^{\mathcal{A}} \notin U_{2^H}$  (P-s-t),  $H^{\mathcal{Q}} \not\models \mathcal{A}$ .  $\Longrightarrow$ : We define  $P = \langle G, \{U_i\}_{i \in |G|} \rangle$  as follows:

- G is the edge extension of G(w) such that  $a^G = a^H$  for  $a \in \{I, \bar{I}\}$  and  $a^G = a^{G(w)}$  for  $a \in \Sigma^{(-)}$ ;
- each set  $U_i \subseteq |\mathcal{A}|$  is defined by:

$$z \in U_i \iff \exists v \in [\mathcal{A}[\_, z]]. \ G(v) \longrightarrow H^{\mathcal{Q}}[\_, [i]_H].$$

Here,  $\mathcal{A}[\_, z]$  denotes the graph  $\mathcal{A}$  in which  $2^{\mathcal{A}}$  has been replaced with z (similarly for  $H^{\mathcal{Q}}[\_, [i]_H]$ ).

Then P is a saturable path for  $\not\models_{REL} w \leq A$ , as follows.

**Sublemma.** Let  $a \in \Sigma_1^{(-, \smile)}$ . If  $G(a) \longrightarrow H^{\mathcal{Q}}[[i]_H, [j]_H]$ , then  $\operatorname{Con}_a^{\mathcal{A}}(U_i, U_j)$ . (Here,  $H^{\mathcal{Q}}[[i]_H, [j]_H]$  denotes the graph  $H^{\mathcal{Q}}$  in which  $1^{H^{\mathcal{Q}}}$  and  $2^{H^{\mathcal{Q}}}$  have been replaced with  $[i]_H$  and  $[j]_H$ , respectively.)

Proof. Let  $z \in U_i$ . By definition, there is  $v \in [\mathcal{A}[\_,z]]$  such that  $G(v) \longrightarrow H^{\mathcal{Q}}[\_,[i]_H]$ . Combining with  $G(a) \longrightarrow H^{\mathcal{Q}}[[i]_H,[j]_H]$  yields  $G(va) \longrightarrow H^{\mathcal{Q}}[\_,[j]_H]$ . Thus, for every  $z' \in \delta_a^{\mathcal{A}}(z), \ z' \in U_j$ . Hence  $\delta_a^{\mathcal{A}}(U_i) \subseteq U_j$ . Similarly by  $G(\widecheck{a}) \longrightarrow H^{\mathcal{Q}}[[j]_H,[i]_H], \ \delta_a^{\mathcal{A}}(U_j) \subseteq U_i$ .

For (P-s-t):  $1^{\mathcal{A}} \in U_{1^G}$  is shown by considering v = 1.  $2^{\mathcal{A}} \not\in U_{2^G}$  is because  $H^{\mathcal{Q}} \not\models \mathcal{A}$ . For (P-Con): Let  $\langle i,j \rangle \in a^G$ . Because  $G(a) \longrightarrow H^{\mathcal{Q}}[[i]_H,[j]_H]$  (since H is a saturation of G), we have  $\mathrm{Con}_a^{\mathcal{A}}(U_i,U_j)$  (the sub-lemma). For (P-Sat): For every  $a \in \Sigma$  and  $i,j \in |G|$ , because either  $G(a) \longrightarrow H^{\mathcal{Q}}[[i]_H,[j]_H]$  or  $G(\overline{a}) \longrightarrow H^{\mathcal{Q}}[[i]_H,[j]_H]$  always holds, we have  $\mathrm{Con}_a^{\mathcal{A}}(U_i,U_j) \vee \mathrm{Con}_{\overline{a}}^{\mathcal{A}}(U_i,U_j)$  (the sub-lemma).  $\square$ 

**Theorem 33.** For two NFAs  $\mathcal{A}, \mathcal{B}$  over  $\Sigma_1^{(-,\smile)}$ , TFAE:

- $\not\models_{REL} A \leq \mathcal{B}$ .
- $\exists w \in [A]$ . there is a saturable path for  $\not\models_{REL} w \leq B$ .

Proof. We have

$$\not\models_{\mathrm{REL}} \mathcal{A} \leq \mathcal{B}$$

$$\iff \exists w \in [\mathcal{A}].\exists H \in \mathcal{S}(G(w)). \ H^{\mathcal{Q}} \not\models \mathcal{A} \leq \mathcal{B} \ (\mathrm{Lem. 21})$$

$$\iff \exists w \in [\mathcal{A}].\exists H \in \mathcal{S}(G(w)). \ H^{\mathcal{Q}} \not\models w \leq \mathcal{B}$$
(Because  $H^{\mathcal{Q}} \models w \ \text{and} \ H^{\mathcal{Q}} \models \mathcal{A} \ \text{by} \ H \in \mathcal{S}(G(w))$ )
$$\iff \exists w \in [\mathcal{A}]. \ \text{there is a saturable path for} \not\models_{\mathrm{REL}} w \leq \mathcal{B}.$$

(Lem. 32) □

## C. Exponential-size model property

The characterization by saturable paths (Thm. 33) gives another bounded model property for ExKA terms (cf. Lem. 21) as follows. The following proof is an analogy of the well-known pumping lemma from automata theory.

**Lemma 34** (Exponential-size model property). For every NFAs  $\mathcal{A}, \mathcal{B}$  over  $\Sigma_{\mathsf{L}}^{(-,\smile)}$ , if  $\not\models_{\mathsf{REL}} \mathcal{A} \leq \mathcal{B}$ , then there is a 2-pointed structure  $\mathfrak{A}$  of size  $\#(|\ddot{\mathfrak{A}}|) \leq \#(|\mathcal{A}|) \times 2^{\#(|\mathcal{B}|)}$  such that  $\ddot{\mathfrak{A}} \not\models_{\mathsf{REL}} \mathcal{A} \leq \mathcal{B}$ .

*Proof.* By Thm. 33, there are a word  $w = a_1 \dots a_n \in [\mathcal{A}]$  and a saturable path  $P = \langle G, \{U_i\}_{i \in [0,n]} \rangle$  for  $\not\models_{\mathrm{REL}} w \leq \mathcal{B}$ . Without loss of generality, we can assume that n is the minimum among such words. Since  $w \in [\mathcal{A}]$ , let  $\{s_i\}_{i \in [0,n]}$  be such that  $\langle s_0, s_n \rangle = \langle 1^{\mathcal{A}}, 2^{\mathcal{A}} \rangle$  and  $s_x \in \delta_{a_i}^{\mathcal{A}}(s_{i-1})$  for  $i \in [n]$ . Assume that  $n+1 > \#(|\mathcal{A}|) \times 2^{\#(|\mathcal{B}|)}$ . By the pigeonhole principle, there are  $0 \leq x < y \leq n$  s.t.  $\langle s_x, U_x \rangle = \langle s_y, U_y \rangle$ . Let  $w' \triangleq a_1 \dots a_x a_{y+1} \dots a_n$ . Let P' be the P in which the source of the edge for  $\langle y, y+1 \rangle \in a_{y+1}^G$  has been replaced with x and the vertices between x+1 and y are removed:

$$P = \bullet \bigcirc a_1 \dots a_x \rightarrow \bullet \bigcirc a_{x+1} \dots a_y \rightarrow \bigcirc a_{y+1} \bullet \bigcirc a_{y+2} \dots a_n \rightarrow \bigcirc \bullet$$

$$U_0 \quad \cdots \quad U_x \qquad \qquad U_y \quad U_{y+1} \quad \cdots \quad U_n$$

$$P' = \bullet \bigcirc a_1 \dots a_x \rightarrow \bullet \bigcirc a_{y+1} \bullet \bigcirc a_{y+2} \dots a_n \rightarrow \bigcirc \bullet$$

$$U_0 \quad \cdots \quad U_x \quad U_{y+1} \quad \cdots \quad U_n$$

(I- or  $\bar{\text{I}}$ -labeled edges and some intermediate vertices are omitted, for simplicity.) Here, when  $\langle x,y+1\rangle\in \text{I}^G$  and  $a_{y+1}=\bar{\text{I}}$ , the graph of P' is not consistent; so, we replace the label I with the label  $\bar{\text{I}}$  for every pair  $\langle i,j\rangle$  s.t.  $i\neq j\wedge \text{Con}_{\bar{\text{I}}}^{\mathcal{B}}(U_i,U_j)$ .  $(i\neq j)$  is for the reflexivity of the relation of I and  $\text{Con}_{\bar{\text{I}}}^{\mathcal{B}}(U_i,U_j)$  is for preserving (P-Con)). Then,  $w'\in [\mathcal{A}]$  holds by  $s_x=s_y$  and P' is an saturable path for  $\not\models_{\text{REL}} w'\leq \mathcal{B}$  because each condition for P' is shown by that for P (with  $U_x=U_y$ ) and that P' is (almost) a "subgraph" of P (see Appendix F, for more details). However, this contradicts that n is the minimum. Thus,  $\#(|G|)=n+1\leq \#(|\mathcal{A}|)\times 2^{\#(|\mathcal{B}|)}$ . Finally,  $\ddot{\mathfrak{U}}=H^{\mathcal{Q}}$  is the desired 2-pointed structure, where H is the saturation of G obtained from Lem. 30.

**Theorem 35.** The equational theory of ExKA terms (w.r.t. binary relations) is decidable in coNEXP.

*Proof.* Similarly for Lem. 22, it suffices to show that the following problem is in NEXP: given ExKA terms t, s, does  $\not\models_{\text{REL}} t \leq s$  hold? By Lem. 34 (with Prop. 26), we can give the following algorithm:

- 1) Take a 2-pointed structure  $\ddot{\mathfrak{A}}$  of size  $\#(|\ddot{\mathfrak{A}}|) \leq \#(|\mathcal{A}_t|) \times 2^{\#(|\mathcal{A}_s|)}$ , non-deterministically. Here,  $\mathcal{A}_t$  and  $\mathcal{A}_s$  are the NFAs obtained from t and s, respectively (Def. 25).
- 2) Return true, if  $\ddot{\mathfrak{A}} \not\models t < s$ ; false, otherwise.

Then  $\not\models_{\text{REL}} t \leq s$ , if some execution returns true;  $\models_{\text{REL}} t \leq s$ , otherwise. Here,  $\ddot{\mathfrak{A}} \not\models t \leq s$  can be decided in exponential time (Prop. 20).

## D. From saturable paths to word automata

For some cases, for an NFA  $\mathcal{A}$ , we can construct an NFA  $\mathcal{A}^{\mathcal{S}}$  such that: for every word w over  $\Sigma_{\mathsf{I}}^{(-,\smile)}\setminus\{\mathsf{I}\}$ , TFAE:

- $w \in [\mathcal{A}^{\mathcal{S}}];$
- there is a saturable path for  $\not\models_{REL} w \leq A$ .

To this end, first, let

$$\varphi(\mathcal{U}, U) \triangleq \bigwedge \begin{cases} U \times (|\mathcal{A}| \setminus U) \times U \times (|\mathcal{A}| \setminus U) \subseteq \mathcal{U} \\ \forall \langle t_1, t_2, t_3, t_4 \rangle \in \mathcal{U}. \forall a \in \Sigma_{\mathbf{I}}. \\ \bigvee \begin{cases} \delta_a^{\mathcal{A}}(t_1) \subseteq U \wedge t_2 \not\in \delta_{\tilde{a}}^{\mathcal{A}}(U) \\ \delta_{\tilde{a}}^{\mathcal{A}}(t_3) \subseteq U \wedge t_4 \not\in \delta_{\tilde{a}}^{\mathcal{A}}(U) \end{cases}$$

and we show the following lemma:

**Lemma 36.** Let  $\mathcal{A}$  be an NFA over  $\Sigma_{\mathsf{I}}^{(-,\smile)}$  and  $w=a_1\ldots a_n$  be a word over  $\Sigma_{\mathsf{I}}^{(-,\smile)}\setminus\{\mathsf{I}\}$ . Recall the formula of (P-Sat):

$$\forall \langle i,j \rangle \in [0,n]^2. \forall a \in \Sigma_{\mathsf{I}}. \bigvee \begin{cases} \delta_a^{\mathcal{A}}(U_i) \subseteq U_j \wedge \delta_{\widecheck{a}}^{\mathcal{A}}(U_j) \subseteq U_i \\ \delta_{\overline{a}}^{\mathcal{A}}(U_i) \subseteq U_j \wedge \delta_{\widecheck{a}}^{\mathcal{A}}(U_j) \subseteq U_i \end{cases}$$

This formula is equivalent to the following formula:8

$$\exists \mathcal{U} \subseteq |\mathcal{A}|^4 . \forall i \in [0, n]. \ \varphi(\mathcal{U}, U_i).$$

Proof. We have

$$\begin{split} & \delta_{a}^{\mathcal{A}}(U_{i}) \subseteq U_{j} \wedge \delta_{\tilde{a}}^{\mathcal{A}}(U_{j}) \subseteq U_{i} \\ & \Leftrightarrow \delta_{a}^{\mathcal{A}}(U_{i}) \subseteq U_{j} \wedge |\mathcal{A}| \setminus U_{i} \subseteq |\mathcal{A}| \setminus \delta_{\tilde{a}}^{\mathcal{A}}(U_{j}) \\ & \Leftrightarrow (\forall t_{1} \in U_{i}.\delta_{a}^{\mathcal{A}}(t_{1}) \subseteq U_{j}) \wedge (\forall t_{2} \in |\mathcal{A}| \setminus U_{i}.t_{2} \notin \delta_{\tilde{a}}^{\mathcal{A}}(U_{j})) \\ & \Leftrightarrow \forall t_{1} \in U_{i}.\forall t_{2} \in |\mathcal{A}| \setminus U_{i}.\delta_{a}^{\mathcal{A}}(t_{1}) \subseteq U_{j} \wedge t_{2} \notin \delta_{\tilde{a}}^{\mathcal{A}}(U_{j}). \end{split}$$

Thus by letting

$$\xi(U) \triangleq \bigvee \begin{cases} \delta_a^{\mathcal{A}}(t_1) \subseteq U \land t_2 \notin \delta_{\check{a}}^{\mathcal{A}}(U) \\ \delta_{\bar{a}}^{\mathcal{A}}(t_3) \subseteq U \land t_4 \notin \delta_{\check{a}}^{\mathcal{A}}(U) \end{cases};$$
$$\nu(U) \triangleq U \times (|\mathcal{A}| \setminus U) \times U \times (|\mathcal{A}| \setminus U),$$

we have

$$\forall \langle i,j \rangle \in [0,n]^{2}. \forall a \in \Sigma_{\mathsf{I}}. \bigvee \begin{cases} \delta_{a}^{\mathcal{A}}(U_{i}) \subseteq U_{j} \wedge \delta_{\tilde{a}}^{\mathcal{A}}(U_{j}) \subseteq U_{i} \\ \delta_{\overline{a}}^{\mathcal{A}}(U_{i}) \subseteq U_{j} \wedge \delta_{\tilde{a}}^{\mathcal{A}}(U_{j}) \subseteq U_{i} \end{cases}$$

$$\Leftrightarrow \forall \langle i,j \rangle \in [0,n]^{2}. \forall a \in \Sigma_{\mathsf{I}}. \forall \langle t_{1},t_{2},t_{3},t_{4} \rangle \in \nu(U_{i}). \ \xi(U_{j})$$

$$\Leftrightarrow \forall \langle t_{1},t_{2},t_{3},t_{4} \rangle \in \bigcup_{i=0}^{n} \nu(U_{i}). \ \forall a \in \Sigma_{\mathsf{I}}. \forall i \in [0,n]. \ \xi(U_{i})$$

$$\Leftrightarrow \exists \mathcal{U} \subseteq |\mathcal{A}|^{4}. \bigcup_{i=0}^{n} \nu(U_{i}) \subseteq \mathcal{U} \quad \wedge \quad \forall \langle t_{1},t_{2},t_{3},t_{4} \rangle \in \mathcal{U}. \forall a \in \Sigma_{\mathsf{I}}. \forall i \in [0,n]. \ \xi(U_{i}) \quad (\diamondsuit)$$

$$\Leftrightarrow \exists \mathcal{U} \subseteq |\mathcal{A}|^{4}. \forall i \in [0,n]. \ \nu(U_{i}) \subseteq \mathcal{U} \quad \wedge \quad \forall \langle t_{1},t_{2},t_{3},t_{4} \rangle \in \mathcal{U}. \forall a \in \Sigma_{\mathsf{I}}. \ \xi(U_{i})$$

$$\Leftrightarrow \exists \mathcal{U} \subseteq |\mathcal{A}|^{4}. \forall i \in [0,n]. \ \varphi(\mathcal{U},U_{i}).$$

<sup>&</sup>lt;sup>8</sup>This transformation is also used for the automata construction in [14] (roughly speaking, the  $\mathcal U$  corresponds to the "P" in [14]), but is a bit more complicated due to converse.

Here, for  $(\diamondsuit)$ ,  $\Longrightarrow$ : By letting  $\mathcal{U} = \bigcup_{i=0}^n \nu(U_i)$ .  $\Longleftrightarrow$ : Because the formula  $\forall \langle t_1, t_2, t_3, t_4 \rangle \in \mathcal{U}'. \forall a \in \Sigma_1. \forall i \in [0, n]. \ \xi(U_i)$ holds for any  $\mathcal{U}' \subseteq \mathcal{U}$  and  $\bigcup_{i=0}^n \nu(U_i) \subseteq \mathcal{U}$ .

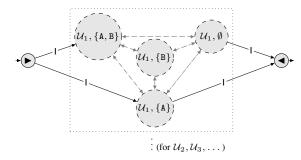
By using the formula of Lem. 36 for (P-Sat), we can check the condition (P-Sat) pointwisely (without considering pairs of  $[0, n]^2$ ). Using this, we give the following NFAs construction:

**Definition 37.** For an NFA  $\mathcal{A}$  over  $\Sigma_{1}^{(-,\smile)}$ , let  $\mathcal{A}^{\mathcal{S}}$  be the NFA over  $\Sigma_{\mathbf{l}}^{(-,\smile)}$  defined by:

- $|\mathcal{A}^{\mathcal{S}}| \stackrel{\cdot}{\triangleq} \{ \blacktriangleright, \blacktriangleleft \} \cup \{ \langle \mathcal{U}, U \rangle \in \wp(|\mathcal{A}|^4) \times \wp(|\mathcal{A}|) \mid \varphi(\mathcal{U}, U) \wedge \varphi(\mathcal{U}, U) = \emptyset \}$  $\delta_{\mathsf{I}}^{\mathcal{A}}(U) \subseteq U$ };
- $I^{A^S}$  is the minimal set such that
  - for all  $\langle \mathcal{U}, U \rangle \in |\mathcal{A}^{\mathcal{S}}|$  s.t.  $1^{\mathcal{A}} \in U$ ,  $\langle \triangleright, \langle \mathcal{U}, U \rangle \rangle \in |\mathcal{A}^{\mathcal{S}}|$ - for all  $\langle \mathcal{U}, \mathcal{U} \rangle \in |\mathcal{A}^{\mathcal{S}}|$  s.t.  $2^{\mathcal{A}} \notin \mathcal{U}$ ,  $\langle \langle \mathcal{U}, \mathcal{U} \rangle$ ,  $\blacktriangleleft \rangle \in \mathsf{I}^{\mathcal{A}^{\mathcal{S}}}$ ;
- for each  $a \in \Sigma_{1}^{(-,\smile)}$ ,  $a^{\mathcal{A}^{\mathcal{S}}}$  is the minimal set such that for every  $\langle \mathcal{U}, U \rangle$ ,  $\langle \mathcal{U}, U' \rangle \in |\mathcal{A}^{\mathcal{S}}|$  s.t.  $\mathrm{Con}_a^{\mathcal{A}}(U, U')$ ,  $\langle \langle \mathcal{U}, U \rangle, \langle \mathcal{U}, U' \rangle \rangle \in a^{\mathcal{A}^{\mathcal{S}}}$  holds; •  $1^{\mathcal{A}^{\mathcal{S}}} = \triangleright$  and  $2^{\mathcal{A}^{\mathcal{S}}} = \blacktriangleleft$ .

(Here,  $\blacktriangleright$  and  $\blacktriangleleft$  are two fresh symbols.  $\mathcal{U}$  is introduced for (P-Sat), cf. Lem. 36. Note that  $\mathcal{U}$  is invariant in transitions.)

For example, when  $|\mathcal{A}| = \{A, B\}$  and  $\langle 1^{\mathcal{A}}, 2^{\mathcal{A}} \rangle = \langle A, B \rangle$ , the NFA  $\mathcal{A}^{\mathcal{S}}$  is of the following form, where the existence of each dashed state  $\langle \mathcal{U}_1, U \rangle$  depends on whether  $\varphi(\mathcal{U}_1, U) \wedge$  $\delta_{\mathbf{l}}^{\mathcal{A}}(U) \subseteq U$  holds and the existence of the a-labeled edge on each dashed edge from  $\langle \mathcal{U}_1, U \rangle$  to  $\langle \mathcal{U}_1, U' \rangle$  depend on whether  $\operatorname{Con}_a^{\mathcal{A}}(U,U')$  holds:



Using this transformation,  $A^{S}$  satisfies the following:

**Lemma 38** (Completeness (of  $A^S$ )). For every NFA A over  $\Sigma_{I}^{(-,\smile)}$  and word w over  $\Sigma_{I}^{(-,\smile)}\setminus\{I\}$ , we have:

 $w \in [\mathcal{A}^{\mathcal{S}}] \iff \text{there is a saturable path for } \not\models_{\text{REL}} w \leq \mathcal{A}.$ 

*Proof.* Let  $w = a_1 \dots a_n$  and  $P = \langle G, \{U_i\}_{i \in [0,n]} \rangle$  be a saturable path for  $\not\models_{\mathrm{REL}} w \leq \mathcal{A}$ . Let  $\mathcal{U} \triangleq \bigcup_{i \in [0,n]} U_i \times U_i$  $(|\mathcal{A}| \setminus U_i) \times U_i \times (|\mathcal{A}| \setminus U_i)$ . Then we have

- $\langle \mathbf{\triangleright}, \langle \mathcal{U}, U_0 \rangle \rangle \in \delta_{\mathsf{I}}^{\mathcal{A}^{\mathcal{S}}}$  (by (P-s-t));
- for all  $i \in [n]$ ,  $\langle \langle \mathcal{U}, U_{i-1} \rangle$ ,  $\langle \mathcal{U}, U_i \rangle \rangle \in \delta_{a_i}^{\mathcal{A}^{\mathcal{S}}}$  (by (P-Con));  $\langle \langle \mathcal{U}, U_n \rangle$ ,  $\blacktriangleleft \rangle \in \delta_{\mathsf{I}}^{\mathcal{A}^{\mathcal{S}}}$  (by (P-s-t)).

Here, for  $i \in [0, n]$ ,  $\langle \mathcal{U}, U_i \rangle \in |\mathcal{A}^{\mathcal{S}}|$  holds, because  $\varphi(\mathcal{U}, U_i)$ holds by (P-Sat) with Lem. 36 and  $\delta_1^{\mathcal{A}}(U_i) \subseteq U_i$  holds by (P-Con). Hence,  $w \in [\mathcal{A}^{\mathcal{S}}]$ .

Lemma 39 (Soundness for the 1<sup>-</sup>-free fragment). For every NFA A over  $\Sigma_{\mathsf{I}}^{(-,\smile)}$  and word w over  $\Sigma_{\mathsf{I}}^{(-,\smile)}\setminus\{\mathsf{I}\}$ , if A does not contain  $I^-$ , then we have:

 $w \in [\mathcal{A}^{\mathcal{S}}] \Longrightarrow \text{there is a saturable path for } \models_{\text{REL}} w \leq \mathcal{A}.$ 

*Proof.* Let  $w = a_1 \dots a_n$ . By the form of  $\mathcal{A}^{\mathcal{S}}$ , there are  $\mathcal{U}$ ,  $U_0, \ldots,$  and  $U_n$  such that

- $\langle \mathbf{\triangleright}, \langle \mathcal{U}, U_0 \rangle \rangle \in \delta_{\mathbf{I}}^{\mathcal{A}^{\circ}};$
- for every  $i \in [n]$ ,  $\langle \langle \mathcal{U}, U_{i-1} \rangle, \langle \mathcal{U}, U_i \rangle \rangle \in \delta_{a_i}^{\mathcal{A}^{\mathcal{S}}}$ ;  $\langle \langle \mathcal{U}, U_n \rangle, \blacktriangleleft \rangle \in \delta_i^{\mathcal{A}^{\mathcal{S}}}$ .

Let H be the I-saturation of G(w) such that

 $\mathsf{I}^H$  is the identity relation.

H is consistent, because G(w) is consistent and  $I^H$  is the identity relation. H is an edge-extension of G(w), because  $\mathsf{I}^H\supseteq \mathsf{I}^{G(w)}=\emptyset$  and  $\bar{\mathsf{I}}^H=|H|^2\setminus \mathsf{I}^H\supseteq \bar{\mathsf{I}}^{G(w)}$ . Hence H is indeed an I-saturation of G(w).

Then  $P = \langle H, \{U_i\}_{i \in [0,n]} \rangle$  is a saturable path for  $\not\models_{REL}$  $w \leq A$  as follows. For (P-s-t): By the definition of  $I^{A^S}$ ,  $1^{\mathcal{A}} \in U_0$  and  $2^{\mathcal{A}} \notin U_n$ . For (P-Con) for  $a \in \Sigma^{(-)}$ : By the definition of  $a_i^{\mathcal{A}^{\mathcal{S}}}$ ,  $\operatorname{Con}_{a_i}^{\mathcal{A}}(U_{i-1}, U_i)$ . (Note that the other edges do not exist.) For (P-Con) for a = 1: Because  $I^H$  is the identity relation and  $U_i \in \delta_1^{\mathcal{A}}(U_i)$  for every  $i \in [0, n]$  (by the definition of  $|\mathcal{A}^{\mathcal{S}}|$ ). For (P-Con) for  $a = \overline{I}$ : Because  $\overline{I}$  does not occur in  $\mathcal{A}$ ,  $\delta_{\bar{i}}^{\mathcal{A}}(U_i) = \emptyset \subseteq U_j$  always holds for every  $i, j \in [0, n]$ . Hence  $\operatorname{Con}_{\overline{1}}^{\mathcal{A}}(U_i, U_j)$ . For (P-Sat): Because  $\mathcal{U}$  satisfies  $\varphi(\mathcal{U}, U_i)$  for every  $i \in [0, n]$  (by the definition of  $|\mathcal{A}^{\mathcal{S}}|$ ), with Lem. 36.  $\square$ 

**Theorem 40.** For every NFAs  $\mathcal{A}, \mathcal{B}$ , over  $\Sigma_1^{(-,\smile)}$ , if  $\mathcal{B}$  does not contain  $I^-$ , then we have

$$\not\models_{\text{REL}} \mathcal{A} \leq \mathcal{B} \iff [\mathcal{A}] \cap [\mathcal{B}^{\mathcal{S}}] \neq \emptyset.$$

Proof. We have

 $\not\models_{\mathrm{REL}} \mathcal{A} \leq \mathcal{B}$ 

 $\iff \exists w \in [\mathcal{A}].$  there is a saturable path for  $\not\models_{REL} w \leq \mathcal{B}.$ (Thm. 33)

$$\iff \exists w \in [\mathcal{A}]. \ w \in [\mathcal{B}^{\mathcal{S}}]$$
 (Lems. 38, 39)

$$\iff [\mathcal{A}] \cap [\mathcal{B}^{\mathcal{S}}] \neq \emptyset.$$

**Theorem 41.** The equational theory of ExKA terms without l⁻ (w.r.t. binary relations) is PSPACE-complete.

*Proof.* For hardness: By Prop. 4, as the term class subsumes  $\mathcal{T}_{\{\cdot,\cup,*\}}$ . For upper bound: Similar to Lem. 22, with (co-)NPSPACE = PSPACE (Savitch's theorem [33]), it suffices to show that the following problem is in NPSPACE: given ExKA terms t, s without  $l^-$ , does  $\not\models_{REL} t \leq s$  hold? By Thm. 40 (with Prop. 26), we can reduce this problem into the emptiness problem of NFAs (of size exponential in the input). Therefore, by using a standard on-the-fly algorithm for the non-emptiness problem of NFAs (which is essentially the graph reachability problem), we can give a non-deterministic polynomial space algorithm.

#### E. Remark on the case of full ExKA terms

Additionally, we remark that the soundness also holds for ExKA terms without complements of term variables.

**Lemma 42** (Soundness for the  $a^-$ -free fragment, cf. Lem. 39). For every NFA A over  $\Sigma_{l}^{(-,\smile)}$  and word w over  $\Sigma_{l}^{(-,\smile)}\setminus\{l\}$ , if w does not contain  $a^{\perp}$  for any  $a \in \Sigma$ , then we have:

 $w \in [\mathcal{A}^{\mathcal{S}}] \Longrightarrow \text{ there is a saturable path for } \not\models_{\text{REL}} w \leq \mathcal{A}.$ 

*Proof.* Let  $w = a_1 \dots a_n$ . By the form of  $\mathcal{A}^{\mathcal{S}}$ , there are  $\mathcal{U}$ ,  $U_0, \ldots,$  and  $U_n$  such that

- $\langle \mathbf{\triangleright}, \langle \mathcal{U}, U_0 \rangle \rangle \in \delta_1^{\mathcal{A}^S};$
- for every  $i \in [n]$ ,  $\langle \langle \mathcal{U}, U_{i-1} \rangle, \langle \mathcal{U}, U_i \rangle \rangle \in \delta_{a_i}^{\mathcal{A}^{\mathcal{S}}}$ ;  $\langle \langle \mathcal{U}, U_n \rangle, \blacktriangleleft \rangle \in \delta_i^{\mathcal{A}^{\mathcal{S}}}$ .

Let H be the I-saturation of G(w) such that

$$\mathsf{I}^H = \{ \langle i, j \rangle \in [0, n]^2 \mid i = j \vee \neg \operatorname{Con}_{\bar{\mathsf{I}}}^{\mathcal{A}}(U_i, U_j) \}.$$

We have  $\operatorname{Con}_{\bar{I}}^{\mathcal{A}}(U_i, U_j) \vee \operatorname{Con}_{\bar{I}}^{\mathcal{A}}(U_i, U_j)$  because  $\mathcal{U}$  satisfies  $\varphi(\mathcal{U}, U_i)$  for every  $i \in [0, n]$  (Lem. 36). If  $\neg \operatorname{Con}_{\bar{i}}^{\mathcal{A}}(U_i, U_i)$ , then  $Con_i^{\mathcal{A}}(U_i, U_i)$ ; thus  $U_i = U_i$ . Therefore, the binary relation  $\{\langle i,j\rangle \in [0,n]^2 \mid \neg \operatorname{Con}_{\bar{1}}^{\mathcal{A}}(U_i,U_j)\}$  is symmetric and transitive; thus  $I^H$  is an equivalence relation. Additionally, His consistent, because  $a^-$  does not occur in H for any  $a \in \Sigma$ . H is an edge-extension of G(w), because  $I^H \supseteq I^{G(w)} = \emptyset$  and  $\overline{\mathsf{I}}^H\supseteq\overline{\mathsf{I}}^{G(w)}$  (by the definition of  $\mathsf{I}^H$ ). Hence H is indeed an I-saturation of G(w).

Then  $P = \langle H, \{U_i\}_{i \in [0,n]} \rangle$  is a saturable path for  $\not\models_{REL}$  $w \leq A$  as follows. For (P-s-t), (P-Sat), and (P-Con) for  $a \in \Sigma^{(-)}$ : Similarly for Lem. 39. For (P-Con) for a = 1: for every  $\langle i,j\rangle\in I^H$ , if i=j, then  $\delta_1^{\mathcal{A}}(U_i)\subseteq U_j$  by the definition of  $|\mathcal{A}^{\mathcal{S}}|$ ; thus  $\operatorname{Con}_{\mathbf{I}}^{\mathcal{A}}(U_i, U_j)$ . If  $\neg \operatorname{Con}_{\bar{\mathbf{I}}}^{\mathcal{A}}(U_i, U_j)$ , then  $Con_{\mathbf{I}}^{\mathcal{A}}(U_i, U_i)$  by (P-Sat). For (P-Con) for  $a = \bar{\mathbf{I}}$ : By the definition of  $I^H$ , we have  $\operatorname{Con}_{\overline{1}}^{\mathcal{A}}(U_i, U_j)$  for every  $\langle i, j \rangle \in [0, n]^2 \setminus \mathsf{I}^H$ .

**Theorem 43.** For every NFAs  $\mathcal{A}, \mathcal{B}$ , over  $\Sigma_{1}^{(-,\smile)}$ , if  $\mathcal{A}$  does not contain  $a^-$  for any  $a \in \Sigma$ , then we have

$$\not\models_{\text{REL}} \mathcal{A} \leq \mathcal{B} \iff [\mathcal{A}] \cap [\mathcal{B}^{\mathcal{S}}] \neq \emptyset.$$

Proof. Cf. Thm. 40 (use Lem. 42 instead of Lem. 39).

**Theorem 44.** The equational theory of ExKA terms without  $a^-$  for any  $a \in \Sigma$  (w.r.t. binary relations) is PSPACE-complete.

However, we leave open the precise complexity of the equational theory of ExKA terms, while it is decidable in coNEXP (Thm. 35) and at least PSPACE-hard (Prop. 4). The problematic case is when both  $I^-$  and  $a^-$  occur. Our automata construction cannot apply to the full case, as follows:

Remark 45 (Failure of the automata construction (Def. 37) for (full) ExKA terms). Consider the soundness (Lems. 39, 42) for ExKA terms: for a given word  $w \in [\mathcal{A}^{\mathcal{S}}]$ , construct a saturable path for  $\not\models_{REL} w \leq A$ . The essence of the proofs in Lems. 39, 42 is that an I-saturation of G(w) always exists. However, for (full) ExKA terms, the situation is changed. For example, let A be the NFA obtained from the term  $a \cup \overline{a}$  (cf. Equation (2)) and  $w = ab\overline{a}$ :

$$\mathcal{A} = \operatorname{Im}_{\bar{\mathbf{I}} \to \bar{\mathbf{O}} \to \bar{\mathbf{I}}} \operatorname{Im}_{\bar{\mathbf{I}} \to \bar{$$

Then  $w \in [\mathcal{A}^{\mathcal{S}}]$  holds because

- $\langle \mathbf{\triangleright}, \langle \mathcal{U}, U_0 \rangle \rangle \in \delta_1^{\mathcal{A}^{\mathcal{S}}};$
- $\langle \langle \mathcal{U}, U_0 \rangle, \langle \mathcal{U}, U_1 \rangle \rangle \in \delta_a^{\mathcal{A}^{\mathcal{S}}};$
- $\langle \langle \mathcal{U}, U_1 \rangle, \langle \mathcal{U}, U_2 \rangle \rangle \in \delta_b^{\mathcal{A}^{\mathcal{S}}}$
- $\langle \langle \mathcal{U}, U_2 \rangle, \langle \mathcal{U}, U_3 \rangle \rangle \in \delta_{\overline{a}}^{\mathcal{A}^{\mathcal{S}}};$
- $\langle \langle \mathcal{U}, U_3 \rangle, \blacktriangleleft \rangle \in \delta_{\mathsf{L}}^{\mathcal{A}^{\mathcal{S}}},$

by letting  $U_0=U_2=\{\mathtt{A},\mathtt{D}\},\ U_1=U_3=\{\mathtt{B},\mathtt{C}\},$  and  $\mathcal{U}=\bigcup_{i\in[0,3]}U_i\times(|\mathcal{A}|\setminus U_i)\times U_i\times(|\mathcal{A}|\setminus U_i).$  However, there does not exist any saturable path for  $\not\models_{REL} w \leq A$ , because  $\models_{\text{REL}} w \leq \mathcal{A}$  (Equation (2)). Additionally, if exists, an Isaturation H of G(w) should satisfy  $(0,2) \in I^H$  (by  $\overline{Ia} \in [A]$ ) and  $\langle 1, 3 \rangle \in I^H$  (by  $a\overline{I} \in [A]$ ) for  $H^Q \not\models A$ :

$$+\underbrace{0}-a \rightarrow \underbrace{1}-b \rightarrow \underbrace{2}-\overline{a} \rightarrow \underbrace{3} \rightarrow .$$

However, H does not satisfy (a-consistent); thus we cannot construct consistent H even if  $w \in [\mathcal{A}^{\mathcal{S}}]$ .

Remark 46. One may think that  $A^{S}$  behaves as a complement of an NFA  $\mathcal{A}$  (cf. Thms. 40, 43). Note that  $\mathcal{A}^{\mathcal{S}}$  is not the language complement of an NFA A, i.e., the following does not hold: for every word  $w, w \in [\mathcal{A}^{\mathcal{S}}] \iff w \notin [\mathcal{A}]$ . E.g., let A be the NFA obtained from the term  $a \cup \overline{a}$  and w = 1:

$$\mathcal{A} = \operatorname{Im}(a) = \operatorname{Im}(w) = \operatorname{$$

By the form of  $\mathcal{A}$ ,  $w \notin [\mathcal{A}]$ . However,  $w \notin [\mathcal{A}^{\mathcal{S}}]$ , as follows. Assume that  $w \in [\mathcal{A}^{\mathcal{S}}]$ . By the form of  $\mathcal{A}^{\mathcal{S}}$ , there are  $\mathcal{U}$  and  $U_0$ such that  $\langle \mathbf{\triangleright}, \langle \mathcal{U}, U_0 \rangle \rangle \in \delta_{\mathbf{I}}^{\mathcal{A}^{\mathcal{S}}}, \ \langle \langle \mathcal{U}, U_0 \rangle, \blacktriangleleft \rangle \in \delta_{\mathbf{J}}^{\mathcal{A}^{\mathcal{S}}}, \ \mathbf{A} \in U_0,$ and  $B \notin U_0$ . By Lem. 36,  $\operatorname{Con}_{\mathcal{A}}^a(U_0, U_0) \vee \operatorname{Con}_{\mathcal{A}}^{\overline{a}}(U_0, U_0)$ . In either case,  $B \in U_0$ , which contradicts  $B \notin U_0$ . Thus  $w \notin [A^S]$ .

# VI. UNDECIDABILITY FOR ECOR\*

A context-free grammar (CFG)  $\mathcal{C}$  over a finite set A is a tuple  $\langle X, \mathcal{R}, \mathsf{s} \rangle$ , where

- X is a finite set of non-terminal labels s.t.  $A \cap X = \emptyset$ ;
- $\mathcal{R}$  is a finite set of rewriting rules  $x \leftarrow w$  of  $x \in X$  and  $w \in (A \cup X)^*$ ;
- $s \in X$  is the *start label*.

The relation  $x \vdash_{\mathcal{C}} w$ , where  $x \in X$  and  $w \in A^*$ , is defined as the minimal relation closed under the following rule: if  $x \leftarrow w_0 x_1 w_1 \dots x_n w_n \in \mathcal{R}$  (where  $x, x_1, \dots, x_n \in X$  and  $w_0, \dots, w_n \in A^*$ ), then  $\frac{x_1 \vdash_{\mathcal{C}} v_1 \dots x_n \vdash_{\mathcal{C}} v_n}{x \vdash_{\mathcal{C}} w_0 v_1 w_1 \dots v_n w_n}.$  The language  $[\mathcal{C}] \subseteq A^*$  is the set  $\{w \mid \mathsf{s} \vdash_{\mathcal{C}} w\}$ . It is well-known that the *universality problem* for CFGs—given a CFG C, does  $[\mathcal{C}] = A^*$  hold?—is  $\Pi_1^0$ -complete.

Let  $\Gamma$  be a set of equations. We write:

$$\mathfrak{A} \models \Gamma \iff \mathfrak{A} \models t = s \text{ for every } t = s \in \Gamma;$$
 
$$\Gamma \models_{\mathrm{REL}} t = s \iff \mathfrak{A} \models t = s \text{ for every } \mathfrak{A} \text{ s.t. } \mathfrak{A} \models \Gamma.$$

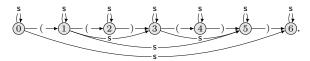
For a CFG  $\mathcal{C} = \langle X, \mathcal{R}, \mathsf{s} \rangle$  and a word  $w = a_1 \dots a_m$ , let  $\Gamma_{\mathcal{C}} \triangleq \{ w \leq x \mid x \leftarrow w \in \mathcal{R} \}$ . Here,  $\ddot{\mathfrak{A}}_{\mathcal{C},w} \triangleq \mathfrak{A}_{\mathcal{C},w}[0,m]$ , where  $\mathfrak{A}_{\mathcal{C},w} \triangleq \langle |\mathfrak{A}|, \{a^{\mathfrak{A}}\}_{a \in A \cup X} \rangle$  is the structure over  $A \cup X$ , defined as follows:

• 
$$|\mathfrak{A}| = [0, m];$$

- for  $a \in A$ ,  $a^{\mathfrak{A}} = \{ \langle i-1, i \rangle \mid i \in [1, m] \text{ and } a_i = a \};$
- the elements of  $\{x^{2i}\}_{x\in X}$  are the minimal relations closed under the following rule: if  $(w_0x_1w_1\dots x_nw_n\leq x)\in\Gamma_{\mathcal{C}}$  (where  $x_1,\dots,x_n\in X$  and  $w_0,\dots,w_n\in A^*$ ), then

$$\frac{\langle i_0, j_0 \rangle \in \llbracket w_0 \rrbracket_{\mathfrak{A}} \quad \langle j_0, i_1 \rangle \in x_1^{\mathfrak{A}} \quad \dots}{\langle j_{n-1}, i_n \rangle \in x_n^{\mathfrak{A}} \quad \langle i_n, j_n \rangle \in \llbracket w_n \rrbracket_{\mathfrak{A}}}{\langle i_0, j_n \rangle \in x^{\mathfrak{A}}}.$$

For example, if  $A = \{(,)\}$ ,  $C = \{\{s\}, \{s \leftarrow (s)s, s \leftarrow I\}, s\}$  (i.e., [C] is the Dyck-1 language), and w = (()()), then  $\mathfrak{A}_{C,w}$  is the following:



Then we have the following:

**Lemma 47.** Let  $C = \langle X, \mathcal{R}, \mathsf{s} \rangle$  be a CFG. For every  $x \in X$  and  $w \in A^*$ , the following are equivalent:

- 1)  $x \vdash_{\mathcal{C}} w$ ;
- 2)  $\ddot{\mathfrak{A}}_{\mathcal{C},w} \models x$ ;
- 3)  $\Gamma_{\mathcal{C}} \models_{\text{REL}} w \leq x$ .

*Proof.*  $1 \Longrightarrow 3$ : By induction on the derivation tree of  $x \vdash_{\mathcal{C}} w$ . This derivation tree is of the following form:  $x_1 \vdash_{\mathcal{C}} v_1 \ldots x_n \vdash_{\mathcal{C}} v_n$ , where  $n \in \mathbb{N}, x_1, \ldots, x_n \in X$ ,  $x_1 \vdash_{\mathcal{C}} w_0 v_1 w_1 \ldots v_n w_n$ , where  $x_1 \vdash_{\mathcal{C}} w_0 v_1 w_1 \ldots v_n w_n \in X$ ,  $x_2 \vdash_{\mathcal{C}} w_0 v_1 w_1 \ldots v_n w_n \in X$ , where  $x_1 \vdash_{\mathcal{C}} w_0 v_1 w_1 \ldots v_n w_n \in X$ , and  $x_1 \vdash_{\mathcal{C}} w_0 x_1 w_1 \ldots x_n w_n \in X$ . W.r.t.  $x_2 \vdash_{\mathcal{C}} w_1 v_1 \ldots v_n w_n \in X$ .

$$w = w_0 v_1 w_1 \dots v_n w_n$$

$$\leq w_0 x_1 w_1 \dots x_n w_n \quad (\Gamma_{\mathcal{C}} \models_{\text{REL}} v_i \leq x_i \text{ for } i \in [n] \text{ (IH)})$$

$$\leq x. \quad ((w_0 x_1 w_1 \dots x_n w_n \leq x) \in \Gamma_{\mathcal{C}})$$

Hence  $\Gamma_{\mathcal{C}} \models_{\text{REL}} w \leq x$ .  $3 \Longrightarrow 2$ : Because  $\mathfrak{A}_{\mathcal{C},w} \models \Gamma_{\mathcal{C}}$  and  $\ddot{\mathfrak{A}}_{\mathcal{C},w} \models w$  hold.  $2 \Longrightarrow 1$ : We show the following:

**Sublemma.** For every  $i, j \in [0, m]$  and  $x \in X$ , if  $\mathfrak{A}_{\mathcal{C}, w}[i, j] \models x$ , then  $i \leq j$  and  $x \vdash_{\mathcal{C}} a_i \dots a_{j-1}$ .

*Proof.* By induction on the derivation tree from the definition of  $\{x^{\mathfrak{A}_{\mathcal{C},w}}\}_{x\in X}$ . This derivation tree is of the follow- $\langle i_0,j_0\rangle\in \llbracket w_0
rbracket_{\mathfrak{A}_{\mathcal{C},w}} \qquad \langle j_0,i_1\rangle\in x_1^{\mathfrak{A}_{\mathcal{C},w}}\qquad\ldots$ 

ing form  $(j_{n-1},i_n) \in x_n^{\mathfrak{A}_{\mathcal{C},w}}$   $(i_n,j_n) \in [\![w_n]\!]_{\mathfrak{A}_{\mathcal{C},w}}$ , where

 $(i_0, j_n) \in x^{\mathfrak{A}_{\mathcal{C}, w}}$   $x_1, \dots, x_n \in X, \ w_0, \dots, w_n \in A^*, \ i_0, j_0, \dots, i_n, j_n \in X$ 

 $x_1, \ldots, x_n \in X$ ,  $w_0, \ldots, w_n \in A^*$ ,  $i_0, j_0, \ldots, i_n, j_n \in [\mathfrak{A}_{\mathcal{C},w}]$ , and  $\langle i_0, j_n \rangle = \langle i, j \rangle$ . By the definition of  $a^{\mathfrak{A}_{\mathcal{C},w}}$  (where  $a \in A$ ), we have  $i_k \leq j_k$  and  $w_k = a_{i_k} \ldots a_{j_{k-1}}$ . By IH, we have  $j_{k-1} \leq i_k$  and  $x_k \vdash_{\mathcal{C}} a_{j_{k-1}} \ldots a_{i_{k-1}}$ . Combining them yields  $i \leq j$  and  $x \vdash_{\mathcal{C}} a_i \ldots a_{j-1}$  (because  $x \leftarrow w_0 x_1 w_1 \ldots x_n w_n \in \mathcal{R}$ ).

By specializing this sub-lemma with  $\langle i,j\rangle=\langle 0,m\rangle$ , this completes the proof.

**Lemma 48.** For every CFG  $\mathcal{C} = \langle X, \mathcal{R}, \mathsf{s} \rangle$ , we have

$$[\mathcal{C}] = A^* \iff \Gamma_{\mathcal{C}} \models_{\mathrm{REL}} A^* \leq \mathsf{s}.$$

(Here,  $A^*$  denotes the term  $(a_1 \cup \cdots \cup a_n)^*$  in the right-hand side, where  $A = \{a_1, \ldots, a_n\}$ .)

Proof. We have

$$[\mathcal{C}] = A^* \iff \forall w \in A^*. \ \mathsf{s} \vdash_{\mathcal{C}} w \qquad \qquad (\text{Def. of []})$$
 
$$\iff \forall w \in A^*. \ \Gamma_{\mathcal{C}} \models_{\text{REL}} w \leq \mathsf{s} \qquad (\text{Lem. 47})$$
 
$$\iff \Gamma_{\mathcal{C}} \models_{\text{REL}} A^* \leq \mathsf{s}. \qquad \Box$$

Additionally, we prepare the following deduction lemma for *Hoare hypotheses*  $u = \bot$  (cf. [34, Thm. 4.1] for KAT):

**Lemma 49.** For every ECoR\* terms t, s, u and every set  $\Gamma$  of equations, we have

$$\Gamma \cup \{u = \bot\} \models_{\text{REL}} t \le s \iff \Gamma \models_{\text{REL}} t \le s \cup (\top u \top).$$

Proof. We have

$$\begin{split} \Gamma \cup \{u = \bot\} &\models_{\mathrm{REL}} t \leq s \\ \iff \text{ for every } \mathfrak{A}[x,y] \text{ s.t. } \mathfrak{A} \models \Gamma \cup \{u = \bot\}, \\ \mathfrak{A}[x,y] \models t \leq s \quad \text{ (Def. of } \models_{\mathrm{REL}} \text{)} \\ \iff \text{ for every } \mathfrak{A}[x,y] \text{ s.t. } \mathfrak{A} \models \Gamma \text{ and } \mathfrak{A}[x,y] \not\models \top u \top, \\ \mathfrak{A}[x,y] \models t \leq s \qquad \qquad (\clubsuit 1) \\ \iff \text{ for every } \mathfrak{A}[x,y] \text{ s.t. } \mathfrak{A} \models \Gamma, \\ \mathfrak{A}[x,y] \models t \leq s \cup (\top u \top) \qquad (\clubsuit 2) \\ \iff \Gamma \models_{\mathrm{REL}} t \leq s \cup (\top u \top). \qquad \text{ (Def. of } \models_{\mathrm{REL}} \text{)} \end{split}$$

Here, (\$1) is because  $\mathfrak{A} \models u = \bot \iff \llbracket u \rrbracket_{\mathfrak{A}} = \emptyset \iff \mathfrak{A}[x,y] \not\models \top u \top$ . (\$2) is because:

$$\begin{split} (\mathfrak{A}[x,y] \not\models \top u \top) \text{ implies } & (\mathfrak{A}[x,y] \models t \leq s) \\ \iff \mathfrak{A}[x,y] \models \top u \top \ \lor \ \mathfrak{A}[x,y] \not\models t \ \lor \ \mathfrak{A}[x,y] \models s \\ \iff \mathfrak{A}[x,y] \not\models t \ \lor \ \mathfrak{A}[x,y] \models s \cup (\top u \top) \\ \iff \mathfrak{A}[x,y] \models t \leq s \cup (\top u \top). \end{split}$$

By Lems. 48, 49, we have the following:

**Theorem 50.** The equational theory of ECoR\* is  $\Pi_1^0$ -complete.

*Proof.* For upper bound: By Lem. 22. For hardness: Let  $C = \langle X, \{x_i \leftarrow w_i \mid i \in [n]\}, \mathsf{s} \rangle$  be a CFG. Then we have

$$\begin{split} [\mathcal{C}] &= A^* \\ \iff \{w_i \leq x_i \mid i \in [n]\} \models_{\text{REL}} A^* \leq \mathsf{s} \qquad \text{(Lem. 48)} \\ \iff \{w_i \cap x_i^- = \bot \mid i \in [n]\} \models_{\text{REL}} A^* \leq \mathsf{s} \\ \text{(For every } \mathfrak{A}, \, \mathfrak{A} \models w_i \leq x_i \iff \mathfrak{A} \models w_i \cap x_i^- = \bot) \\ \iff \models_{\text{REL}} A^* \leq \mathsf{s} \cup \left(\bigcup_{i=1}^n \top (w_i \cap x_i^-) \top\right) \qquad \text{(Lem. 49)} \\ \iff \models_{\text{REL}} A^* \leq \mathsf{s} \cup \left(\bigcup_{i=1}^n (a \cup a^-)(w_i \cap x_i^-)(a \cup a^-)\right). \\ \text{(} \models_{\text{REL}} \top = a \cup a^-, \text{ where } a \text{ is some element in } A.) \end{split}$$

Thus we can reduce the universality problem for CFGs, which is  $\Pi^0_1$ -hard, to the equational theory of ECoR\* (precisely,  $\mathcal{T}_{\{\cdot,\cup,\cap,\underline{\ }^*\}}$  with the complement of term variables).

## VII. CONCLUSION AND FUTURE WORK

We have studied the computational complexity of existential calculi of relations with transitive closure, using edge saturations. A natural interest is to extend our complexity results for more general syntaxes. We believe that the upper bound results for intersection-free fragments hold even if we extend them with *tests* in KAT (by considering *guarded strings* [35] instead of words (strings), in saturable paths); e.g., *KAT with top* (w.r.t. binary relations), which are recently studied for modeling *incorrectness logic* [24], [25], [36], [37].

Another future work is to study the axiomatizability of them. Unfortunately, the equational theory of (full) ECoR\* is not finitely axiomatizable because it is not recursively enumerable (Thm. 50); but we leave it open to finding some complete (finite) axiomatization for its fragments, including KA terms with complements of term variables. (The equation (1) indicates that, at least, we need axioms of KA with top w.r.t. binary relations [24].)

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#### APPENDIX A

PROOF OF THE EQUATIONS IN THE INTRODUCTION

(The notations in this section depend on Sect. III-A.) For Equation (1):  $\models_{\text{REL}} \top = a \cup a^{-}$ . For every structure  $\mathfrak{A}$  and  $x, y \in |\mathfrak{A}|$ , we have

$$\begin{split} \langle x,y\rangle \in [\![\top]\!]_{\mathfrak{A}} &\iff \mathsf{true} \\ &\iff \langle x,y\rangle \in [\![a]\!]_{\mathfrak{A}} \vee \langle x,y\rangle \not\in [\![a]\!]_{\mathfrak{A}} \\ &\iff \langle x,y\rangle \in [\![a\cup a^-]\!]_{\mathfrak{A}}. \end{split}$$

For Equation (2):  $\models_{\text{REL}} aba^- \leq \mathsf{I}^-a^- \cup a\mathsf{I}^-$ . Assume  $\langle x_0, x_3 \rangle \in \llbracket aba^- \rrbracket_{\mathfrak{A}}$ . Let  $x_1$  and  $x_2$  be s.t.  $\langle x_0, x_1 \rangle \in \llbracket a \rrbracket_{\mathfrak{A}}$ ,  $\langle x_1, x_2 \rangle \in \llbracket b \rrbracket_{\mathfrak{A}}$ , and  $\langle x_2, x_3 \rangle \in \llbracket a^- \rrbracket_{\mathfrak{A}}$ . Because  $\langle x_0, x_1 \rangle \in a^{\mathfrak{A}}$  and  $\langle x_2, x_3 \rangle \notin a^{\mathfrak{A}}$ ,  $\langle x_0, x_1 \rangle \neq \langle x_2, x_3 \rangle$  should hold. We distinguish the following cases:

- If  $x_0 \neq x_2$ , then  $\langle x_0, x_2 \rangle \in \llbracket \mathsf{I}^- \rrbracket_{\mathfrak{A}}$  and  $\langle x_2, x_3 \rangle \in \llbracket a^- \rrbracket_{\mathfrak{A}}$ . Thus,  $\langle x_0, x_3 \rangle \in \llbracket \mathsf{I}^- a^- \cup a \mathsf{I}^- \rrbracket_{\mathfrak{A}}$ .
- Otherwise  $(x_1 \neq x_3)$ ,  $\langle x_0, x_1 \rangle \in \llbracket a \rrbracket_{\mathfrak{A}}$  and  $\langle x_1, x_3 \rangle \in \llbracket I^- \rrbracket_{\mathfrak{A}}$ . Thus,  $\langle x_0, x_3 \rangle \in \llbracket I^- a^- \cup a I^- \rrbracket_{\mathfrak{A}}$ .

This completes the proof.

For Equation (3):  $\models_{\text{REL}} a \leq \mathsf{I}^- \cup aa$ . Assume  $\langle x,y \rangle \in \llbracket a \rrbracket_{\mathfrak{A}}$ . We distinguish the following cases:

- If  $x \neq y$ , then  $\langle x, y \rangle \in [\![ I^- ]\!]_{\mathfrak{A}}$ . Thus,  $\langle x, y \rangle \in [\![ I^- \cup aa ]\!]_{\mathfrak{A}}$ .
- Otherwise (x=y),  $\langle x,y\rangle \in [a]_{\mathfrak{A}}$ , y=x, and  $\langle x,y\rangle \in [a]_{\mathfrak{A}}$ . Thus,  $\langle x,y\rangle \in [1^- \cup aa]_{\mathfrak{A}}$ .

This completes the proof.

For Equation (4):  $\models_{\text{REL}} a \ \ a^- \le \mathsf{I}^-$ . Assume  $\langle x_0, x_2 \rangle \in [\![a \ \ \ ]\!]_{\mathfrak{A}}$ . Let  $x_1$  be s.t.  $\langle x_0, x_1 \rangle \in [\![a \ \ \ ]\!]_{\mathfrak{A}}$  and  $\langle x_1, x_2 \rangle \in [\![a \ \ \ ]\!]_{\mathfrak{A}}$ . Because  $\langle x_1, x_0 \rangle \in a^{\mathfrak{A}}$  and  $\langle x_1, x_2 \rangle \not\in a^{\mathfrak{A}}$ ,  $x_0 \ne x_2$  should hold. Thus, we have  $\langle x_0, x_2 \rangle \in [\![\mathfrak{I}^-]\!]_{\mathfrak{A}}$ . This completes the proof.

#### APPENDIX B

Note: Supplement of Footnote 4

Let  $\mathcal{T}_{\mathrm{gen}}$  be the set of terms defined as follows:

$$\mathcal{T}_{\text{gen}} \ni t, s, u ::= a \mid a^- \mid \mathbf{I} \mid \mathbf{I}^- \mid \bot \mid \bot^- \mid \top \mid \top^- \mid t \cdot s \mid t \cup s \mid t^* \mid t^{\smile} \qquad (a \in \Sigma)$$

The binary relation  $[\![t]\!]_{\mathfrak{A}}\subseteq |\mathfrak{A}|^2$  of an  $\mathcal{T}_{\mathrm{gen}}$  term t on a structure  $\mathfrak{A}$  is defined as follows, where  $a\in\Sigma$  and  $b\in\Sigma\cup\{\mathsf{I},\bot,\top\}$ :

$$\begin{bmatrix} a \end{bmatrix}_{\mathfrak{A}} \triangleq a^{\mathfrak{A}} \qquad \qquad \begin{bmatrix} b^- \end{bmatrix}_{\mathfrak{A}} \triangleq (b^-)^{\mathfrak{A}} \\
 \begin{bmatrix} \bot \end{bmatrix}_{\mathfrak{A}} \triangleq \emptyset \qquad \qquad \begin{bmatrix} \top \end{bmatrix}_{\mathfrak{A}} \triangleq |\mathfrak{A}|^2 \\
 \begin{bmatrix} t \cup s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cup [s]_{\mathfrak{A}} \qquad \qquad \begin{bmatrix} t \cap s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cap [s]_{\mathfrak{A}} \\
 \begin{bmatrix} t \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} \qquad \qquad \begin{bmatrix} t \cap s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cap [s]_{\mathfrak{A}} \\
 \begin{bmatrix} t \cdot s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cdot [s]_{\mathfrak{A}} \qquad \qquad \begin{bmatrix} t \cap s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cap [s]_{\mathfrak{A}} \\
 \begin{bmatrix} t \cap s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cap [s]_{\mathfrak{A}} \cap [s]_{\mathfrak{A}} \\
 \begin{bmatrix} t \cap s \end{bmatrix}_{\mathfrak{A}} \triangleq [t]_{\mathfrak{A}} \cap [s]_{\mathfrak{A}} \cap$$

We write  $\models_{\text{REL}} t = s$  if  $[\![t]\!]_{\mathfrak{A}} = [\![s]\!]_{\mathfrak{A}}$  for every structure  $\mathfrak{A}$ . The *equational theory over* S *w.r.t. binary relations* is defined

as the set of every pairs t=s of terms in  $\mathcal{T}_S$  s.t.  $\models_{\mathrm{REL}} t=s$ . We use the notation  $\models$  (Notation 2) also for  $\mathcal{T}_{\mathrm{gen}}$ .

For term  $t \in \mathcal{T}_{gen}$ , the converse normal form  $\check{t}$  (e.g., [23, Sect. 2.1]) of the term  $t^{\smile}$  is defined by:

$$\breve{a} \triangleq a \qquad \qquad (a \in \Sigma^{(-)})$$

$$\breve{a} \triangleq a \qquad \qquad a \stackrel{\smile}{=} \triangleq a \qquad (a \in \{\mathsf{I},\mathsf{I}^-,\mathsf{T},\mathsf{T}^-,\bot,\bot^-\})$$

$$\widecheck{t \cdot s} \triangleq \breve{s} \cdot \breve{t} \qquad (\widecheck{t \cdot s}) \stackrel{\smile}{=} \triangleq \widecheck{t} \stackrel{\smile}{=} \cdot \widecheck{s} \stackrel{\smile}{=}$$

$$\widecheck{t}^* \triangleq (\widecheck{t})^* \qquad (\widecheck{t}^*) \stackrel{\smile}{=} \triangleq (\widecheck{t}^{\smile})^*$$

$$\widecheck{t \cup s} \triangleq \widecheck{t} \cup \widecheck{s} \qquad (\widecheck{t \cup s}) \stackrel{\smile}{=} \triangleq \widecheck{t} \stackrel{\smile}{=} \cup \widecheck{s} \stackrel{\smile}{=}$$

$$(\widecheck{t}^{\smile}) \stackrel{\smile}{=} \triangleq \widecheck{t} .$$

**Proposition 51.** For every term  $t \in \mathcal{T}_{gen}$ ,  $\models_{REL} \check{t} = t^{\smile}$ .

*Proof Sketch.* By straightforward induction on t. For example, if  $t = s \cdot u$ , for every  $\mathfrak{A}[x, y]$ , we have

$$\mathfrak{A}[x,y] \models \widecheck{s \cdot u} \iff \mathfrak{A}[x,y] \models \widecheck{u} \cdot \widecheck{s} \qquad \text{(Def. of } \widecheck{\bullet}\text{)}$$

$$\iff \exists z. \ \mathfrak{A}[x,z] \models \widecheck{u} \ \land \ \mathfrak{A}[z,y] \models \widecheck{s} \qquad \text{(Def. of } []]\text{)}$$

$$\iff \exists z. \ \mathfrak{A}[x,z] \models u^{\smile} \ \land \ \mathfrak{A}[z,y] \models s^{\smile} \qquad \text{(IH)}$$

$$\iff \mathfrak{A}[x,y] \models u^{\smile} \cdot s^{\smile} \qquad \text{(Def. of } []]\text{)}$$

$$\iff \mathfrak{A}[x,y] \models (u \cdot s)^{\smile}. \qquad \text{(Def. of } []]\text{)}$$

**Proposition 52.** The equational theory of  $\mathcal{T}_{gen}$  can be reduced to that of ECoR\* in polynomial time.

*Proof.* Let t and s be terms in  $\mathcal{T}_{\mathrm{gen}}$ . Let t' (resp. s') be the term  $\check{t}$  (resp.  $\check{s}$ ) in which each  $\top^-$  has been replaced with  $\bot$  and each  $\bot^-$  has been replaced with  $\top$ . Then,  $\models_{\mathrm{REL}} t = s \iff \models_{\mathrm{REL}} t' = s'$  by Prop. 51 with  $\models_{\mathrm{REL}} \top^- = \bot$  and  $\models_{\mathrm{REL}} \bot^- = \top$ . By the construction, t' and s' can be obtained from t and s in polynomial time, respectively. Also, t' and s' are  $\mathcal{T}_{\mathrm{gen}}$  terms, because  $\smile$  only applies to  $a \in \Sigma^{(-)}$  and  $\top^-$  and  $\bot^-$  does not occur.

# APPENDIX C NOTE: PROOF OF PROPS. 8, 9

**Proposition 53.** For every structure  $\mathfrak{A}$  and graphs G, H,

$$[G \cap H]_{\mathfrak{A}} = [G]_{\mathfrak{A}} \cap [H]_{\mathfrak{A}}$$
 (Prop. 53\cdot)  

$$[G \cdot H]_{\mathfrak{A}} = [G]_{\mathfrak{A}} \cdot [H]_{\mathfrak{A}}$$
 (Prop. 53\cdot)  

$$[G^{\smile}]_{\mathfrak{A}} = [G]_{\mathfrak{A}}^{\smile}.$$
 (Prop. 53\sucdet)

*Proof.* Prop. 53 $\cap$ . By the definition of  $[]_{\mathfrak{A}}$  (Def. 7), it suffices to show that for every  $x, y \in |\mathfrak{A}|$ :

$$\exists f. \ f \colon (G \cap H) \longrightarrow \mathfrak{A}[x,y]$$
 
$$\iff \exists f_G, f_H. \ f_G \colon G \longrightarrow \mathfrak{A}[x,y] \land f_H \colon H \longrightarrow \mathfrak{A}[x,y].$$

 $\implies$ : By letting  $f_G = \{\langle x', f(x') \rangle \mid x' \in |G| \}$  and  $f_H = \{\langle x', f(x') \rangle \mid x' \in |H| \}$ .  $\iff$ : By letting  $f = f_G \cup f_H$ . Note

that  $f_G(1^G) = x = f_H(1^H)$  and  $f_G(2^G) = y = f_H(2^H)$  by Def. 7; so f is indeed a map.

Prop. 53. By the definition of  $[]_{\mathfrak{A}}$ , it suffices to show that for every  $x, y \in |\mathfrak{A}|$ :

$$\exists f. \ f \colon (G \cdot H) \longrightarrow \mathfrak{A}[x,y]$$

$$\iff \exists z, f_G, f_H. \ f_G: G \longrightarrow \mathfrak{A}[x, z] \land f_H: H \longrightarrow \mathfrak{A}[z, y].$$

 $\implies$ : By letting  $z=f(2^G), f_G=\{\langle x',f(x')\rangle \mid x'\in |G|\}$ , and  $f_H=\{\langle x',f(x')\rangle \mid x'\in |H|\}$ .  $\iff$ : By letting  $f=f_G\cup f_H$ . Note that  $f_G(2^G)=z=f_H(1^H)$  by Def. 7; so f is indeed a map.

Prop. 53 $\smile$ . By the definition of  $[]_{\mathfrak{A}}$ , it suffices to show that for every  $x, y \in |\mathfrak{A}|$ :

$$\exists f. \ f: G^{\smile} \longrightarrow \mathfrak{A}[x,y] \iff \exists f_G. \ f_G: G \longrightarrow \mathfrak{A}[y,x].$$

This is clear by using the same map.

**Proposition 54** (restatement of Prop. 8). For every structure  $\mathfrak{A}$  and PCoR\* term t, we have  $[\![t]\!]_{\mathfrak{A}} = [\![\mathcal{G}(t)]\!]_{\mathfrak{A}}$ .

*Proof.* By induction on t.

Case t = a where  $a \in \Sigma$ : For every  $x, y \in |\mathfrak{A}|$ , we have

$$\begin{split} \langle x,y\rangle \in [\![a]\!]_{\mathfrak{A}} &\iff \langle x,y\rangle \in a^{\mathfrak{A}} & \text{(Def. of } [\![]\!]) \\ &\iff \bullet \circ - a \to \circ \bullet & \longrightarrow \mathfrak{A}[x,y] \\ &\iff \langle x,y\rangle \in [\![ \bullet \circ - a \to \circ \bullet \ ]\!]_{\mathfrak{A}} & \text{(Def. 7)} \\ &\iff \langle x,y\rangle \in [\![\mathcal{G}(a)]\!]_{\mathfrak{A}}. & \text{(Def. of } \mathcal{G}) \end{split}$$

Case t = I: For every  $x, y \in |\mathfrak{A}|$ , we have

Case t = T: For every  $x, y \in |\mathfrak{A}|$ , we have

Case  $t = \bot$ : For every  $x, y \in |\mathfrak{A}|$ , we have

$$\langle x,y \rangle \in \llbracket \bot \rrbracket_{\mathfrak{A}} \iff \mathsf{false} \qquad \qquad \mathsf{(Def. of } \llbracket \rrbracket \mathsf{)} \\ \iff \langle x,y \rangle \in \llbracket \emptyset \rrbracket_{\mathfrak{A}} \qquad \qquad \mathsf{(Def. 7)} \\ \iff \langle x,y \rangle \in \llbracket \mathcal{G}(\bot) \rrbracket_{\mathfrak{A}}. \qquad \mathsf{(Def. of } \mathcal{G} \mathsf{)}$$

Case  $t = s \cdot u$ :

 $= [\![ \mathcal{G}(s \cdot u) ]\!]_{\mathfrak{A}}.$ 

$$\begin{split} & \llbracket s \cdot u \rrbracket_{\mathfrak{A}} = \llbracket s \rrbracket_{\mathfrak{A}} \cdot \llbracket u \rrbracket_{\mathfrak{A}} & \text{(Def. of } \llbracket \rrbracket) \\ & = \llbracket \mathcal{G}(s) \rrbracket_{\mathfrak{A}} \cdot \llbracket \mathcal{G}(u) \rrbracket_{\mathfrak{A}} & \text{(IH)} \\ & = \bigcup_{G \in \mathcal{G}(s)} \bigcup_{H \in \mathcal{G}(u)} \llbracket G \rrbracket_{\mathfrak{A}} \cdot \llbracket H \rrbracket_{\mathfrak{A}} & \text{($\cdot$ is distributive w.r.t. } \cup ) \\ & = \bigcup_{G \in \mathcal{G}(s)} \bigcup_{H \in \mathcal{G}(u)} \llbracket G \cdot H \rrbracket_{\mathfrak{A}} & \text{(Equation (Prop. 53$\cdot))} \end{split}$$

(Def. of  $\mathcal{G}$ )

Case  $t = s \cap u$ :

$$\begin{split} & \llbracket s \cap u \rrbracket_{\mathfrak{A}} = \llbracket s \rrbracket \cap \llbracket u \rrbracket & \text{(Def. of } \llbracket \rrbracket \text{)} \\ & = \llbracket \mathcal{G}(s) \rrbracket_{\mathfrak{A}} \cap \llbracket \mathcal{G}(u) \rrbracket_{\mathfrak{A}} & \text{(IH)} \\ & = \bigcup_{G \in \mathcal{G}(s)} \bigcup_{H \in \mathcal{G}(u)} \llbracket G \rrbracket_{\mathfrak{A}} \cap \llbracket H \rrbracket_{\mathfrak{A}} & \text{(} \cap \text{ is distributive w.r.t. } \cup \text{)} \\ & = \bigcup_{G \in \mathcal{G}(s)} \bigcup_{H \in \mathcal{G}(u)} \llbracket G \cap H \rrbracket_{\mathfrak{A}} & \text{(Equation (Prop. 53 \cap))} \\ & = \llbracket \mathcal{G}(s \cap u) \rrbracket_{\mathfrak{A}}. & \text{(Def. of } \mathcal{G} \text{)} \end{split}$$

Case  $t = s \cup u$ :

$$[s \cup u]_{\mathfrak{A}} = [s]_{\mathfrak{A}} \cup [u]_{\mathfrak{A}}$$
 (Def. of [])
$$= [\mathcal{G}(s)]_{\mathfrak{A}} \cup [\mathcal{G}(u)]_{\mathfrak{A}}$$
 (IH)
$$= [\mathcal{G}(s) \cup \mathcal{G}(u)]_{\mathfrak{A}}$$

$$= [\mathcal{G}(s \cup u)]_{\mathfrak{A}}.$$
 (Def. of  $\mathcal{G}$ )

Case  $t = s^*$ :

**Proposition 55** (restatement of Prop. 9). For every PCoR\* terms, t and s, we have

$$\models_{\text{REL}} t \leq s \iff \forall G \in \mathcal{G}(t).\exists H \in \mathcal{G}(s). \ H \longrightarrow G.$$

*Proof.* By the following formula transformation:

$$\begin{split} &\models_{\mathrm{REL}} t \leq s \iff \forall \mathfrak{A}. \ \llbracket t \rrbracket_{\mathfrak{A}} \subseteq \llbracket s \rrbracket_{\mathfrak{A}} & (\mathrm{Def.\ of} \models_{\mathrm{REL}}) \\ &\iff \forall \mathfrak{A}. \ \llbracket \mathcal{G}(t) \rrbracket_{\mathfrak{A}} \subseteq \llbracket \mathcal{G}(s) \rrbracket_{\mathfrak{A}} & (\mathrm{Prop.\ 8}) \\ &\iff \forall \mathfrak{A}. \forall G \in \mathcal{G}(t). \ \llbracket G \rrbracket_{\mathfrak{A}} \subseteq \bigcup_{H \in \mathcal{G}(s)} \llbracket H \rrbracket_{\mathfrak{A}} & (\mathrm{Def.\ of}\ \llbracket \rrbracket) \\ &\iff \forall G \in \mathcal{G}(t). \forall \mathfrak{A}. \ \llbracket G \rrbracket_{\mathfrak{A}} \subseteq \bigcup_{H \in \mathcal{G}(s)} \llbracket H \rrbracket_{\mathfrak{A}} & (\mathrm{Def.\ of}\ \llbracket \rrbracket) \\ &\iff \forall G \in \mathcal{G}(t). \forall \ddot{\mathfrak{A}}. & (G \longrightarrow \ddot{\mathfrak{A}}) \text{ implies } (\exists H \in \mathcal{G}(s). H \longrightarrow \ddot{\mathfrak{A}}) & (\mathrm{Def.\ of}\ \llbracket \rrbracket) \\ &\iff \forall G \in \mathcal{G}(t). \exists H \in \mathcal{G}(s). H \longrightarrow G. & (\heartsuit) \end{split}$$

Here, for  $(\heartsuit)$ ,  $\Longrightarrow$ : Let  $\ddot{\mathfrak{A}}$  be the saturation (see Sect. IV-B) of G s.t.

- $a^{\ddot{\mathfrak{A}}} = a^G$  for  $a \in \Sigma$ ; •  $I^{\mathfrak{A}} = \{\langle x, x \rangle \mid x \in |\mathfrak{A}|\}.$
- $(\ddot{\mathfrak{A}}$  is a 2-pointed structure, because  $\overline{a}^{\ddot{\mathfrak{A}}}=|\ddot{\mathfrak{A}}|^2\setminus a^{\ddot{\mathfrak{A}}}$  and  $|\ddot{\mathfrak{A}}|$ is the identity relation.) Since  $G \longrightarrow \ddot{\mathfrak{A}}$  by the identity map, there is some  $H \in \mathcal{G}(s)$  s.t.  $H \longrightarrow \ddot{\mathfrak{A}}$  (by the assumption). Because  $a^H = \emptyset$  for every  $a \in \Sigma_1^{(-)} \setminus \Sigma$  (note that s is positive) and  $a^{\ddot{\mathfrak{A}}}=a^G$  for every  $a\in \Sigma$ , we have  $H\longrightarrow G$  by the same homomorphism for  $H \longrightarrow \ddot{\mathfrak{A}}$ .  $\Longleftarrow$ : Let  $H \in \mathcal{G}(s)$ be s.t.  $H \longrightarrow G$ . Let  $\ddot{\mathfrak{A}}$  be any 2-pointed structure s.t.  $G \longrightarrow$  $\mathfrak{A}$ . Then, by transitivity of  $\longrightarrow$ , we have  $H \longrightarrow \mathfrak{A}$ . Hence,  $\exists H \in \mathcal{G}(s). \ H \longrightarrow \mathfrak{A}.$

# APPENDIX D Proof of Prop. 11

**Proposition 56** (restatement of Prop. 11). For every structure  $\mathfrak{A}$  and ECoR\* term t, we have  $[t]_{\mathfrak{A}} = [\mathcal{G}(t)]_{\mathfrak{A}}$ .

*Proof.* By induction on t, as with Prop. 8.

Case t = a where  $a \in \Sigma_{1}^{(-)} \setminus \Sigma_{1}$ :

$$\begin{split} \langle x,y\rangle \in [\![a]\!]_{\mathfrak{A}} &\iff \langle x,y\rangle \in a^{\mathfrak{A}} & \text{(Def. of } [\![]\!]) \\ &\iff \bullet \bigcirc -a \longrightarrow \circ \bullet & \longrightarrow \mathfrak{A}[x,y] \\ &\iff \langle x,y\rangle \in [\![ \ \, \bullet \bigcirc -a \longrightarrow \circ \bullet \ ]\!]_{\mathfrak{A}} & \text{(Def. 7)} \\ &\iff \langle x,y\rangle \in [\![\mathcal{G}(a)]\!]_{\mathfrak{A}}. & \text{(Def. of } \mathcal{G}) \end{split}$$

For the other cases, they are in the same way as the proof of Prop. 8.

# APPENDIX E PROOF COMPLETION OF PROP. 26

**Proposition 57.** For every ExKA term u and structure  $\mathfrak A$  over  $\Sigma$ , we have

$$\llbracket u \rrbracket_{\mathfrak{A}} = \bigcup_{w \in [u]} \llbracket w \rrbracket_{\mathfrak{A}}.$$

Here,  $[u] \subseteq (A_{\mathsf{I}}^{(-,\smile)}\setminus\{\mathsf{I}\})^*$  is the language of u over  $A_{\mathsf{I}}^{(-,\smile)}\setminus\{\mathsf{I}\}$  obtained by viewing u as a term over  $A_{\mathsf{I}}^{(-,\smile)}\setminus\{\mathsf{I}\}$ .

*Proof.* By induction on u. Case u=a for  $a\in A_{\mathsf{I}}^{(-,\smile)}$  (including  $a=\mathsf{I}$ ): Since [a]= $\{a\}$ , we have  $\llbracket a \rrbracket_{\mathfrak{A}} = \bigcup_{w \in [a]} \llbracket w \rrbracket_{\mathfrak{A}}$ .

Case  $u = \bot$ : Since  $[\bot] = \emptyset$ , we have  $[\![\bot]\!]_{\mathfrak{A}} = \emptyset =$  $\bigcup_{w \in \emptyset} \llbracket w \rrbracket_{\mathfrak{A}} = \bigcup_{w \in [\bot]} \llbracket w \rrbracket_{\mathfrak{A}}.$ Case  $u = t \cup s$ :

$$\begin{aligned}
&[t \cup s]_{\mathfrak{A}} = [t]_{\mathfrak{A}} \cup [s]_{\mathfrak{A}} \\
&= (\bigcup_{w \in [t]} [w]_{\mathfrak{A}}) \cup (\bigcup_{w \in [s]} [w]_{\mathfrak{A}}) \\
&= \bigcup_{w \in [t] \cup [s]} [w]_{\mathfrak{A}} \\
&= \bigcup_{w \in [t \cup s]} [w]_{\mathfrak{A}}.
\end{aligned} (IH)$$

Case  $u = t \cdot s$ :

$$\begin{split} &\llbracket t \cdot s \rrbracket_{\mathfrak{A}} = \llbracket t \rrbracket_{\mathfrak{A}} \cdot \llbracket s \rrbracket_{\mathfrak{A}} \\ &= (\bigcup_{w \in [t]} \llbracket w \rrbracket_{\mathfrak{A}}) \cdot (\bigcup_{v \in [s]} \llbracket v \rrbracket_{\mathfrak{A}}) \\ &= \bigcup_{w \in [t], v \in [s]} (\llbracket w \rrbracket_{\mathfrak{A}} \cdot \llbracket v \rrbracket_{\mathfrak{A}}) \qquad \text{(By distributivity)} \\ &= \bigcup_{w \in [t], v \in [s]} \llbracket wv \rrbracket_{\mathfrak{A}} \\ &= \bigcup_{w \in [t \cdot s]} \llbracket w \rrbracket_{\mathfrak{A}}. \end{split}$$

Case  $u = t^*$ : We have

$$\begin{split} \llbracket t^* \rrbracket_{\mathfrak{A}} &= \bigcup_{n \in \mathbb{N}} \llbracket t^n \rrbracket_{\mathfrak{A}} = \bigcup_{n \in \mathbb{N}} \llbracket t \rrbracket_{\mathfrak{A}}^n \\ &= \bigcup_{n \in \mathbb{N}} (\bigcup_{w \in [t]} \llbracket w \rrbracket_{\mathfrak{A}})^n \qquad \qquad \text{(IH)} \\ &= \bigcup_{n \in \mathbb{N}} \bigcup_{w_1, \dots, w_n \in [t]} (\llbracket w_1 \rrbracket_{\mathfrak{A}} \cdot \dots \cdot \llbracket w_n \rrbracket_{\mathfrak{A}}) \\ &= \bigcup_{n \in \mathbb{N}} \bigcup_{w_1, \dots, w_n \in [t]} \llbracket w_1 w_2 \dots w_n \rrbracket_{\mathfrak{A}} \\ &= \bigcup_{n \in \mathbb{N}} \bigcup_{w \in [t^n]} \llbracket w \rrbracket_{\mathfrak{A}} = \bigcup_{w \in [t^*]} \llbracket w \rrbracket_{\mathfrak{A}}. \qquad \Box \end{split}$$

#### APPENDIX F

#### PROOF COMPLETION OF LEM. 34

Proof completion of Lem. 34 (P' is an saturable path). Let

$$\langle l_0, \dots, l_x, l_{x+1}, \dots, l_{n'} \rangle = \langle 0, \dots, x, y+1, \dots, n \rangle.$$

(Here, " $y+1,\ldots,n$ " is the empty sequence if y=n.) Then,  $w' = a_{l_0} \dots a_{l_{n'}}$  holds and  $P' = \langle G', \{U'_i\}_{i \in [0,n']} \rangle$  is as follows:

- $U'_{i} = U_{l_{i}}$ , for each  $i \in [0, n']$ ;
- G' is the I-saturation of G(w') such that  $I^{G'} = \{\langle i, j \rangle \in \mathcal{C} \mid G' = \{\langle i, j \rangle \in \mathcal{C} \mid$  $[0, n']^2 \mid i = j \vee \neg \operatorname{Con}_{\bar{\mathsf{l}}}^{\mathcal{B}}(U_i', U_j') \}.$

If  $\neg \operatorname{Con}_{\bar{1}}^{\mathcal{B}}(U_i', U_j')$ , then  $\operatorname{Con}_{\bar{1}}^{\mathcal{B}}(U_i', U_j')$  (by (P-Sat) for P); thus  $U_i' = U_j'$ . Therefore, the binary relation  $\{\langle i, j \rangle \in [0, n]^2 \mid$  $\neg \operatorname{Con}_{\bar{1}}^{\mathcal{B}}(U_i', U_i')$  is symmetric and transitive; thus  $I^{G'}$  is an equivalence relation. G' is consistent because G is consistent. (In particular, when  $\langle x, y+1 \rangle \in I^G$  and  $a_{y+1} = \overline{I}$ , we have  $U_x=U_y$  (by the definition of x and y) and  $U_x=U_{y+1}$  (by  $\langle x,y+1\rangle\in \mathsf{I}^G$ ), thus  $\mathrm{Con}_{\bar{\mathsf{I}}}^{\mathcal{B}}(U_x',U_{x+1}')$  (since  $a_{y+1}=\bar{\mathsf{I}}$  with (P-Con) for P). Hence,  $\langle x,x+1\rangle\in \bar{\mathsf{I}}^{G'}$ . Thus, since  $a_{y+1}=\bar{\mathsf{I}}$ , G' is consistent.) G' is an edge-extension of G(w), because  $\mathsf{I}^{G'}\supseteq \mathsf{I}^{G(w)}=\emptyset$  and  $\bar{\mathsf{I}}^{G'}\supseteq \bar{\mathsf{I}}^{G(w)}$  (by the definition of  $\mathsf{I}^{G'}$ ). Hence, G' is indeed an I-saturation of G(w).

We show that P' is an saturable path for  $\not\models_{REL} w' \leq \mathcal{B}$ .

- $\bullet$  For (P-s-t): By  $U_0'=U_0$  and  $U_{n'}'=U_n$  with (P-s-t) for P.
- For (P-Con):
  - for a=1: Let  $\langle i,j\rangle\in \mathsf{I}^{G'}$ . If i=j, then we have  $\mathrm{Con}_{\bar{\mathsf{I}}}^{\mathcal{B}}(U_i',U_j')$  by (P-Con) for P. If  $\neg\,\mathrm{Con}_{\bar{\mathsf{I}}}^{\mathcal{B}}(U_i',U_j')$ , then we have  $\mathrm{Con}_{\bar{\mathsf{I}}}^{\mathcal{B}}(U_i',U_j')$  by (P-Sat) for P.
  - for  $a = \overline{I}$ : By the definition of  $I^{G'}$ .
- For  $\operatorname{Con}_{a_{l_i}}^{\mathcal{B}}(U'_{i-1},U'_i)$  where  $i\in[n']$ :  $\operatorname{Case}\ i\neq x+1 \colon \operatorname{By}\ \operatorname{Con}_{a_{l_i}}^{\mathcal{B}}(U'_{i-1},U'_i) \ (\operatorname{since}\ \langle l_{i-1},l_i\rangle \in a_{l_i}^G \ \operatorname{with}\ (\operatorname{P-Con}) \ \operatorname{for}\ P).$   $\operatorname{Case}\ i=x+1 \colon \operatorname{Then},\ U'_x=U_{l_x}=U_x=U_y \ \operatorname{and}\ U'_{x+1}=U_{l_{x+1}}=U_{y+1}. \ \operatorname{By}\ \operatorname{Con}_{a_y}^{\mathcal{B}}(U_y,U_{y+1}) \ (\operatorname{since}\ \langle y,y+1\rangle \in a_y^G \ \operatorname{with}\ (\operatorname{P-Con}) \ \operatorname{for}\ P), \ \operatorname{we}\ \operatorname{have}\ \operatorname{Con}_{a_{l_{x+1}}}^{\mathcal{B}}(U'_x,U'_{x+1}).$
- For (P-Sat): By  $\{U_i'\mid i\in [0,n']\}\subseteq \{U_i\mid i\in [0,n]\}$  with (P-Sat) for P.

Hence, P' is an saturable path for  $\not\models_{REL} w' \leq \mathcal{B}$ .