The Monadic Quantifier Alternation Hierarchy over Grids and Graphs

Oliver Matz*, Nicole Schweikardt**, Wolfgang Thomas*

Abstract

The monadic second-order quantifier alternation hierarchy over the class of finite graphs is shown to be strict. The proof is based on automata theoretic ideas and starts from a restricted class of graph-like structures, namely finite two-dimensional grids. Considering grids where the width is a function of the height, we prove that the difference between the levels $k+1$ and k of the monadic hierarchy is witnessed by a set of grids where this function is $(k+1)$-fold exponential. We then transfer the hierarchy result to the class of directed (or undirected) graphs, using an encoding technique called "strong reduction".

It is notable that one can obtain sets of graphs which occur arbitrarily high in the monadic hierarchy but are already definable in the first-order closure of existential monadic second-order logic. We also verify that these graph properties even belong to the complexity class NLOG, which indicates a profound difference between the monadic hierarchy and the polynomial hierarchy.

1 Introduction

The subject of this paper is monadic second-order logic over graphs. In this logic, one can quantify over vertices and sets of vertices; typical properties which are formalizable in monadic logic are k-colourability and connectivity.

Monadic second-order graph properties can be classified by the alternation depth of set quantifiers which occur in defining formulas. One speaks of a Σ_k-formula (Π_k-formula) if its prenex normal form has a prefix of k alternating blocks of set quantifiers starting with an existential (universal) block, followed by a first-order kernel.

Fagin [Fag95] raised the question whether for increasing k the monadic Σ_k-formulas allow to define more and more properties of finite graphs. This question is the "monadic analogue" of the problem whether the polynomial

*RWTH Aachen, Lehrstuhl für Informatik VII, 52056 Aachen, email: {matz|thomas}@informatik.rwth-aachen.de

**Johannes Gutenberg-Universität Mainz, Institut für Informatik / FB 17, 55099 Mainz, email: nisch@informatik.uni-mainz.de

hierarchy (of complexity theory) is infinite; in the context of finite graphs the k-th level of the polynomial hierarchy is given by the graph properties which are definable by general Σ_k-formulas where second-order quantifiers may range also over relations of arity higher than 1.

As partial results on Fagin's problem we mention his result [Fag75] (see also [FSV95]) that connectivity of graphs is a monadic property which is not Σ_1 (i.e., not definable by a Σ_1-formula). In [Sch94], Schwentick extended this result to graphs with built-in order. Within the range of monadic Σ_1-formulas, Otto [Ott95] showed that the length of the (single) block of leading existential set quantifiers induces a strict hierarchy of properties. From automata theory (cf. Büchi [Büc60], Elgot [Elg61], and subsequent work), it is also known that over words and trees (considered as special labelled graphs), all monadic second-order properties are in fact Σ_1-properties; in [Tho82] it was observed that even a single existential set quantifier suffices. Considering coloured grids as underlying models, a compression of existential second-order prefixes to a single existential quantifier was obtained in [Mat98b].

In the present paper we show that over finite graphs in general, the Σ_k-formulas induce a strict hierarchy of graph properties, thus answering Fagin's question affirmatively.

A main idea of the proof is to consider rectangular grids instead of graphs. (At a later point we transfer the hierarchy theorem from the domain of grids back to the domain of graphs.) A grid of size (m, n) is, roughly speaking, a finite graph whose vertices are arranged as elements of a $(m \times n)$-matrix and which has two edge relations corresponding to vertical and horizontal successors. For a function $f : \mathbb{N} \to \mathbb{N}$ let L_f be the set of grids of size $(m, f(m))$ for $m \geqslant 1$. The levels of the monadic hierarchy are separated by such sets L_f: We show that for a Σ_k-definable set L_f, the function f can be at most k-fold exponential, whereas for each $k \geqslant 1$, a k-fold exponential function f exists such that L_f is Σ_k-definable.

For the first claim (which proves the desired lower bound on expressiveness of Σ_k-formulas), we give two proofs. The first uses an automata theoretic view of formulas as developed in [GRST96], which is then applied in the spirit of [Gia94] (Section 3 below). In [GRST96] it was shown that a Σ_1-formula over grids can be transformed into a nondeterministic acceptor, called "tiling system", which roughly consists of a list of state quadruples. A "run" of such a tiling system associates a state with each grid vertex such that any resulting 2×2 array of states occurs as a quadruple in the tiling system. If there are k states and only grids of height m are considered as inputs, a tiling system can be viewed as a finite automaton which scans a grid column by column, each of which is assigned one of k^m "column states". So, by the standard pumping lemma, the shortest grid of height m accepted by the automaton cannot be longer than k^m. For the grids in a Σ_1-definable set L_f one infers that their width grows at most by a single exponential in their height m. Using the well-known powerset and projection construction for finite automata $k-1$ times, one proves that for a Σ_k-definable set L_f, the function f can be at most k-fold exponential.

Instead of invoking [GRST96], one may base the needed pumping arguments on an appropriate version of the Ehrenfeucht-Fraïssé game. In Section 3.2 below, we give a self-contained presentation of this alternative approach.

For the second claim, namely that for a suitable k-fold exponential function f one can exhibit a Σ_k-definition of L_f, a counting process up to $f(m)$ is described within grids of height m, which will enforce their width to be $f(m)$. We obtain (in Section 4) even sharpened results by providing both a Σ_k- and a Π_k-definition of this counting process.

To obtain the main result, the hierarchy result is transferred from the domain of grids to the domain of graphs (Section 5). For this purpose we apply the well-known technique of interpretations in a version called "strong first-order reductions" here, refining the monadic first-order reductions of [Cos93]. We proceed in two steps and introduce corresponding encodings: from coloured grids to directed graphs and from directed graphs to undirected graphs.

The hierarchy result on the monadic hierarchy can be refined in analogy to the situation as known from the classical hierarchies of recursion theory. Let us denote by $\underline{\Sigma_k}$ and $\underline{\Pi_k}$ the classes of graph properties (say of undirected graphs) which are definable by monadic formulas with second-order Σ_k-prefix, respectively Π_k-prefix. Then for $k \geqslant 1$, the classes $\underline{\Sigma_k}$ and $\underline{\Pi_k}$ are incomparable and strictly included in the Boolean closure of $\underline{\Sigma_k}$, which itself is strictly included in $\underline{\Delta_{k+1}} := \underline{\Sigma_{k+1}} \cap \underline{\Pi_{k+1}}$, which in turn is strictly included in $\underline{\Sigma_{k+1}}$ and $\underline{\Pi_{k+1}}$.

Our witness sets of undirected graphs (or of coloured grids) for the levels of the monadic hierarchy can all be defined with very moderate use of set quantifiers. We show that these witness sets belong to the closure of the class Σ_1 under first-order quantification. This slightly extends the result of [AFS98] which puts these witness sets into the class "closed monadic NP" (where defining formulas have a quantifier prefix consisting of first-order quantifiers and existential set quantifiers in any order). We even show that these witness sets are definable in the extension of first-order logic by the unary transitive closure operator and hence belong to the complexity class NLOG. So NLOG contains instances beyond any given level of the monadic hierarchy, whereas it is well-known that any level of the monadic hierarchy also contains problems which are complete for the corresponding level of the polynomial hierarchy. So one has to conclude that the two hierarchies show profound differences and that the present results do not provide any progress for the problem whether the polynomial hierarchy is infinite.

A more feasible project would be to investigate the hierarchy built upon "closed monadic NP" of [AFS98]. Here one allows "first-order quantifications for free", i.e. formulas with quantifier prefixes in which both first-order and monadic second-order quantifiers occur but where the classification into levels refers only to the second-order quantifiers. It is open whether in this generalized context the alternation depth of the second-order quantifiers again induces a strict hierarchy. Further open questions are listed in the Conclusion.

In [Mat98a], both the definability and the non-definability results have been extended. In particular, is is shown that if a set L_f of grids is definable in the closure of Σ_k under first-order quantifications, then the function f is at most $(k+1)$-fold exponential. (This had been shown in [AFS98] for the case $k = 1$.) On the other hand, a particular $(k+1)$-fold exponential function is definable in this class of formulas.

The present paper combines and extends results of the two conference contributions [MT97] and [Sch97]. In the first, the strictness of the monadic hierarchy over graphs was shown, based on the infinity of the monadic hierarchy over grids, and in the second even over grids the monadic hierarchy was proved to be strict.

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2 Notation and Results

2.1 Graphs and Grids

The signature of graphs $\tau_{\text{Graph}} = \{E\}$ contains a binary relation symbol E. A (finite, directed) *graph* is a finite τ_{Graph}-structure, i.e. a pair $(\text{dom}G, E^G)$ with $E^G \subseteq (\text{dom}G)^2$. If E^G is irreflexive and symmetric, we call G *undirected.*

A central role in this paper is played by a variant of graphs, called grids. Here we consider the signature $\tau_{\text{Grid}} = \{S_1, S_2\}$ containing the binary "successor" relation symbols S_1 and S_2. The elements of a grid are, for some $m, n \geqslant 1$, the pairs (i, j) with $i \in \{1, \ldots, m\}$ and $j \in \{1, \ldots, n\}$; so, writing $[n]$ for $\{1, \ldots, n\}$, the universe of a grid is of the form $[m, n] := [m] \times [n]$. The *grid of height m and width n* is the τ_{Grid}-structure

$$\underline{[m, n]} := ([m, n], S_1^{m,n}, S_2^{m,n}),$$

where $S_1^{m,n}$ and $S_2^{m,n}$ are the "vertical" and the "horizontal" successor relations on $[m, n]$, containing all pairs $((i, j), (i + 1, j))$, respectively all pairs $((i, j), (i, j + 1))$ from $[m, n]$.

The expressions *row, column, top, bottom* etc. are interpreted as in the terminology of matrices; e.g. the leftmost column contains exactly the vertices $(i, 1)$ for $1 \leqslant i \leqslant m$, and the top row consists of all vertices $(1, j)$ for $1 \leqslant j \leqslant n$.

We also consider grids whose vertices are labelled by t-bit vectors (for some $t \geqslant 0$). Such a labelling determines a t-tuple of subsets of vertices (such that the i-th subset contains the vertices whose label vector has 1 in its i-th component). Accordingly, we adjoin unary predicate symbols $X_1, \ldots, X_t$ to the signature of grids, obtaining the signature $\tau_{t\text{-Grid}} = \tau_{\text{Grid}} \cup \{X_1, \ldots, X_t\}$. A *$t$-bit grid* (for some $t \geqslant 0$) is a $\tau_{t\text{-Grid}}$-structure, i.e. of the form $R = (\text{dom}R, S_1^R, S_2^R, X_1^R, \ldots, X_t^R)$ whose restriction to τ_{Grid} is a grid. So grids are 0-bit grids.

A different version of grids is obtained via the signature $\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\}$ with binary relation symbols $\leqslant_1, \leqslant_2$. In this context, a grid is considered as the structure

$$([m,n], S_1^{m,n}, S_2^{m,n}, \leqslant_1^{m,n}, \leqslant_2^{m,n}),$$

where $\leqslant_1^{m,n} = \{((i,j),(i',j)) \in [m,n] \times [m,n] \mid i \leqslant i'\}$, and $\leqslant_2^{m,n} = \{((i,j),(i,j')) \in [m,n] \times [m,n] \mid j \leqslant j'\}$. We write "$x <_i y$" as abbreviation for "$x \leqslant_i y \wedge \neg x = y$", for $i \in \{1,2\}$.

The classes of graphs, undirected graphs, grids, and t-bit grids will be denoted Graph, UGraph, Grid, and t-Grid, respectively.

2.2 Monadic Second-Order Logic

Let τ be a relational signature. We use $x, y, x_1, x_2, \ldots$ as first-order variables and $X, Y, C, \ldots$ as monadic second-order variables, the latter officially numbered as $X_1, X_2, \ldots$. *Monadic second-order formulas over τ* (MSO-formulas for short) are built up as usual from atomic formulas $x = y$, Xy, and $r(x_1, \ldots, x_l)$ (for an l-ary relation symbol r of τ) by means of the propositional connectives and first- and second-order quantifications. *First-order formulas* over τ (FO-formulas for short) are MSO-formulas in which no second-order quantifier occurs.

The set of variables occurring free in a formula φ is denoted free(φ). If free(φ) $\subseteq \{X_1, \ldots, X_t, x_1, \ldots, x_m\}$, we sometimes write $\varphi(X_1, \ldots, X_t, x_1, \ldots, x_m)$. If M is a τ-structure and $U_1, \ldots, U_t$ and $u_1, \ldots, u_m$ are subsets, respectively elements, of the domain dom$M$ of M, and if $\varphi(X_1, \ldots, X_t, x_1, \ldots, x_m)$ is a formula over τ, then we write $M \models \varphi[U_1, \ldots, U_t, u_1, \ldots, u_m]$ to indicate that φ is true in M under the assignment that maps X_i to U_i and x_j to u_j for all i, j. If $\mathcal{C}$ is a class of τ-structures and φ is a sentence, i.e., free(φ) $= \emptyset$, then we write $Mod_{\mathcal{C}}(\varphi)$ for the set $\{M \in \mathcal{C} \mid M \models \varphi\}$ of models of φ. In the context of t-bit grids, an MSO-formula φ with free(φ) $\subseteq \{X_1, \ldots, X_t\}$ is considered as a sentence over $\tau_{t\text{-Grid}}$.

By $\text{FO}^{\text{TC}(1)}$ we denote the class of first-order formulas together with the unary TC-operator (see e.g. [EF95]). So $\text{FO}^{\text{TC}(1)}$-formulas are built up from atomic formulas using propositional connectives, first-order quantifications, and the rule that if $\varphi(x, y, z_1, \ldots, z_n)$ is an $\text{FO}^{\text{TC}(1)}$-formula, then

$\mathrm{TC}(x, y, \varphi)$ is also an $\mathrm{FO}^{\mathrm{TC}(1)}$-formula, with the set $\{x, y\} \cup \mathrm{free}(\varphi)$ of free variables. The satisfaction relation $M \models \mathrm{TC}(x, y, \varphi)[u, v, w_1, \ldots w_n]$ holds iff there are elements $u_0, \ldots, u_m$ for some $m \geqslant 0$ such that $u = u_0$, $v = u_m$, and $M \models \varphi[u_i, u_{i+1}, w_1, \ldots, w_n]$ for all $i < m$.

2.3 Alternation Hierarchies

For the subsequent definitions fix a relational signature τ. We use the following convention:

A class $\mathcal{F}$ of formulas is *closed under first-order quantifications* (respectively *Boolean combinations*, respectively *existential monadic second-order quantifications*) iff whenever φ, ψ are in $\mathcal{F}$, then so are $\exists x\varphi$ and $\forall x\varphi$ (respectively $\varphi \vee \psi$ and $\neg\varphi$, respectively $\exists X\varphi$).

Let Σ_0 (and $\mathrm{closed}(\Sigma_0)$) be the set of first-order formulas, and let $\Sigma_0^{\mathrm{TC}(1)} = \mathrm{FO}^{\mathrm{TC}(1)}$.

For every $k \geqslant 0$, we denote by Σ_{k+1} the smallest set of formulas that contains all negations of formulas in Σ_k and is closed under existential monadic second-order quantification. Π_k denotes the set of negations of formulas in Σ_k.

For every $k \geqslant 0$, we denote by $\mathrm{closed}(\Sigma_{k+1})$ the smallest set of formulas that contains all negations of formulas in $\mathrm{closed}(\Sigma_k)$ and is closed under first-order quantification and existential monadic second-order quantification.

In other words, $\mathrm{closed}(\Sigma_k)$ contains formulas in prenex normal form where the quantifier prefix contains an interleaving of unary second-order quantifiers and first-order quantifiers such that when we ignore the (universal and existential) first-order quantifiers there are at most $k-1$ alternations of existential and universal monadic second-order quantifier blocks, starting with an existential one.

For every $k \geqslant 0$, we denote by $\Sigma_{k+1}^{\mathrm{TC}(1)}$ the smallest set of formulas that contains all negations of formulas in $\Sigma_k^{\mathrm{TC}(1)}$ and is closed under existential monadic second-order quantification.

So $\Sigma_k^{\mathrm{TC}(1)}$ contains formulas in prenex normal form that have a Σ_k-prefix of monadic second-order quantifiers and a kernel in which first-order quantifiers and the unary TC-operator are admitted.

By $\mathrm{B}(\mathcal{F})$ (respectively $\mathrm{PFO}(\mathcal{F})$, respectively $\mathrm{FO}(\mathcal{F})$) we denote, for every class $\mathcal{F}$ of formulas, the smallest superset of $\mathcal{F}$ that is closed under Boolean combinations (respectively under first-order quantifications, respectively under both of these operations). These classes are called the *Boolean closure of $\mathcal{F}$*, *positive first-order closure of $\mathcal{F}$*, and *first-order closure of $\mathcal{F}$*, respectively.

We now turn to the classes of properties which are definable by formulas with the restrictions above: For a set $\mathcal{F}$ of formulas and a class $\mathcal{C}$ of τ-

structures, let

$$\underline{\mathcal{F}}(\mathcal{C}) = \{L \subseteq \mathcal{C} \mid Mod_{\mathcal{C}}(\varphi) = L \text{ for some sentence } \varphi \text{ in } \mathcal{F}\}$$

be the class of all subsets of $\mathcal{C}$ definable by sentences in $\mathcal{F}$.

Given a class $\mathcal{C}$, the class $\underline{\Sigma_k}(\mathcal{C})$ is called "*the k-th level of the monadic quantifier alternation hierarchy*" over $\mathcal{C}$. Furthermore one sets $\underline{\Delta_k}(\mathcal{C}) = \underline{\Sigma_k}(\mathcal{C}) \cap \underline{\Pi_k}(\mathcal{C})$. The lowest level $\underline{\Sigma_1}(\mathcal{C})$ is sometimes called "monadic NP" (over $\mathcal{C}$). Where in [AFS98] the expressions *first-order closure of monadic NP* and *closed monadic NP* are used, we shall speak of the *first-order closure of* $\underline{\Sigma_1}$ and *closed* $\underline{\Sigma_1}$, respectively.

In Section 4 below we employ "Σ_k-formulas", "FO(Σ_k)-formulas", etc., in a more liberal meaning, namely for formulas which (over the class of structures under consideration) are equivalent to Σ_k-formulas, FO(Σ_k)-formulas, etc.

Let us summarize some known facts on the introduced hierarchies. The k-th level of the monadic second-order hierarchy contains properties that are complete for the k-th level of the polynomial hierarchy. This has been shown in [AFS98] for the class of graphs and in [Sch97] for the class of coloured grids. It also has been mentioned (without proof) in [MP96]. Assuming that the polynomial hierarchy is strict, this would imply the strictness of the monadic second-order hierarchy.

In [AFS98] it has been shown, using a special form of Ehrenfeucht-Fraïssé games, that $\underline{\Sigma_1}$(UGraph) is properly included in $\underline{\mathrm{FO}(\Sigma_1)}$(UGraph) and in $\underline{\mathrm{closed}(\Sigma_1)}$(UGraph); moreover, the latter class contains properties which do not belong to the former. Also it is noted there that every $\Sigma_k^{\mathrm{TC}(1)}$-definable property is closed(Σ_k)-definable, and every closed(Σ_k)-definable property belongs to the k-th level of the polynomial hierarchy.

As Ajtai, Fagin, and Stockmeyer point out in [AFS98], the levels of the monadic hierarchy, in particular the existential fragment, are not sufficiently robust since they are not even closed under first-order quantifications, whereas the levels of the polynomial hierarchy, the origin of interest, are. This motivates a study of the closed hierarchy. In contrast to the strictness of the monadic hierarchy (as proved in this paper), it is open whether the "closed hierarchy" can be shown to be strict (without the assumption of the strictness of the polynomial hierarchy).

2.4 Results

Our main results are the following two:

Theorem 1 *If $\mathcal{C}$ is the class of grids, directed graphs, or undirected graphs, and if $k \geqslant 1$, then*

$$\underline{\mathrm{B}(\Sigma_k)}(\mathcal{C}) \subsetneqq \underline{\Delta_{k+1}}(\mathcal{C}).$$

Moreover, if $\mathcal{C}$ is the class of directed graphs or undirected graphs, then for $k \geqslant 1$ the classes $\underline{\Sigma_k}(\mathcal{C})$ and $\underline{\Pi_k}(\mathcal{C})$ are incomparable.

The first claim strengthens the result of [MT97], which says $\underline{\Sigma_k}(\text{Graph}) \subsetneqq \underline{\Sigma_{k+1}}(\text{Graph})$ and the result of [Sch97], which says $\underline{\Sigma_k}(\text{Grid}) \subsetneqq \underline{\Delta_{k+1}}(\text{Grid})$.

By elementary rules of quantifier logic (see also Remark 21) one concludes the following:

Corollary 2 *If $\mathcal{C}$ is the class of directed graphs or undirected graphs, then for $k \geqslant 1$ the following inclusion diagram is valid (where lines indicate strict inclusions):*

$$\begin{tikzcd}[column sep=small]
\underline{\Sigma_{k+1}}(\mathcal{C}) \arrow[dr, dash] & & \underline{\Pi_{k+1}}(\mathcal{C}) \arrow[dl, dash] \\
& \underline{\Delta_{k+1}}(\mathcal{C}) \arrow[d, dash] & \\
& \underline{\mathrm{B}(\Sigma_k)}(\mathcal{C}) \arrow[dl, dash] \arrow[dr, dash] & \\
\underline{\Sigma_k}(\mathcal{C}) & & \underline{\Pi_k}(\mathcal{C})
\end{tikzcd}$$

A closer inspection of the formulas that witness the hierarchy gives the following non-inclusion results, which show that already variants of Σ_1-formulas allow to define sets arbitrarily high in the monadic hierarchy.

Theorem 3 *For every $k \geqslant 1$,*

$$\underline{\Sigma_1^{\mathrm{TC}(1)}}(\text{Grid}) \not\subseteq \underline{\Sigma_k}(\text{Grid}) \qquad \textit{and} \qquad \underline{\text{closed}(\Sigma_1)}(\text{Grid}) \not\subseteq \underline{\Sigma_k}(\text{Grid}),$$

and if $\mathcal{C}$ is the class of graphs or undirected graphs, then

$$\underline{\mathrm{FO}^{\mathrm{TC}(1)}}(\mathcal{C}) \not\subseteq \underline{\Sigma_k}(\mathcal{C}) \qquad \textit{and} \qquad \underline{\mathrm{PFO}(\Sigma_1)}(\mathcal{C}) \not\subseteq \underline{\Sigma_k}(\mathcal{C}).$$

The main work for the proof of these results is done in Sections 3 and 4, concentrating on the class of grids. In Section 5 we will transfer these results from grids to graphs to get Theorems 1 and 3.

The basis of Theorem 1 are definability results for sets of grids. For a function $f : \mathbb{N} \to \mathbb{N}$ we denote by L_f the set of grids whose size is $(m, f(m))$ for $m \geqslant 1$. We say that a formula φ over τ_{Grid} *defines* the function $f : \mathbb{N} \to \mathbb{N}$ iff $Mod_{\text{Grid}}(\varphi) = L_f$. A function f is called *at most k-fold exponential* if $f(m)$ is $s_k(\mathcal{O}(m))$, where $s_0(m) = m$ and $s_{k+1}(m) = 2^{s_k(m)}$ for every $m \geqslant 1$, $k \geqslant 0$. If $f(m)$ is $s_k(\Theta(m))$, then f is called *k-fold exponential.*

In Section 3 we will show:

Theorem 4 *Every* $\mathrm{B}(\Sigma_k)$*-definable function is at most k-fold exponential.*

Then, in Section 4, we will show:

Theorem 5 *Let* $f_1(m) := 2^m, \quad f_{k+1}(m) := f_k(m)2^{f_k(m)}$ *for* $m, k \geqslant 1$. *For every* $k \geqslant 1$*, the function* f_k *is definable*

1. *in* Σ_k *and in* Π_k *over* τ_{Grid}*,*
2. *in* Σ_1 *and in* Π_1 *over* $\tau_{\mathrm{Grid}} \cup \{\leqslant_1, \leqslant_2\}$*,*
3. *in* $\Sigma_1^{\mathrm{TC}(1)}$ *and in* $\Pi_1^{\mathrm{TC}(1)}$ *over* τ_{Grid}*,*
4. *by a sentence of the form* $\exists \overline{X}\psi$ *and by a sentence of the form* $\forall \overline{X}\psi'$*, where* $\overline{X}$ *is a monadic second-order variable tuple and* $\psi \in \mathrm{PFO}(\Sigma_1)$ *and* $\psi' \in \mathrm{PFO}(\Pi_1)$ *over* τ_{Grid}*.*

The claims of Theorems 1 and 3 about the class of grids follow immediately from Theorems 4 and 5, because f_{k+1} is not at most k-fold exponential. The claims of Theorem 1 and 3 about the classes of graphs and of undirected graphs will be deduced in Section 5.

Further results on growth rates of functions definable in the first-order closure of the k-th level of the monadic hierarchy can be found in [Mat98a]: every $\mathrm{FO}(\Sigma_k)$-definable function is at most $(k+1)$-fold exponential and there is a $(k+1)$-fold exponential function definable in $\mathrm{PFO}(\Sigma_k)$. These results imply some more separation results, in particular $\underline{\mathrm{FO}(\Sigma_k)}(\mathcal{C}) \subsetneq \underline{\mathrm{FO}(\Sigma_{k+1})}(\mathcal{C})$ if $\mathcal{C}$ is the class of grids or graphs.

3 Bounds of Growth Rate of MSO-definable Functions

The aim of this section is to prove Theorem 4. In order to verify a limited expressive power of formulas, using combinatorial arguments, we take an automata theoretic view of formulas. In this context it is convenient to view coloured grids as matrices over a finite alphabet, here called "pictures".

Definition 6 *A* picture of size (m, n) *(where* $m, n \geqslant 1$*) over an alphabet* Γ *is a* $m{\times}n$*-matrix over* Γ*, i.e. a mapping* $[m, n] \to \Gamma$*. The set of pictures of size* (m, n) *over* Γ *is denoted by* $\Gamma^{m,n}$*. The set of pictures of arbitrary size over* Γ *is denoted by* $\Gamma^{+,+}$*. A subset of* $\Gamma^{+,+}$ *is called a* picture language over Γ.

The picture associated to a t-bit grid $R = (\mathrm{dom}R, S_1^R, S_2^R, X_1^R, \ldots, X_t^R)$ *is the* $m{\times}n$*-matrix* P *over alphabet*[1] $\{0,1\}^t$ *where, for each* $1 \leqslant l \leqslant t$*, the* l*-th component of* $P(i,j)$ *is* 1 *iff* $(i,j) \in X_l^R$*. The picture language (over alphabet* $\{0,1\}^t$*)* defined by *a formula* φ *with free variables among* $X_1, \ldots, X_t$ *(or, equivalently, by a sentence of signature* $\tau_{t\text{-Grid}}$*) is the set of pictures associated to models of* φ*. A picture language is* Σ_k-definable *iff it is definable by a* Σ_k*-formula.*

[1] We adopt the convention that $\{0,1\}^0$ is some singleton alphabet.

If φ is a formula with free(φ) $\subseteq \{X_1, \ldots, X_t\}$, we write $Mod_t(\varphi)$ for the set of pictures over $\{0,1\}^t$ that are associated to t-bit grids in $Mod_{t\text{-Grid}}(\varphi)$.

By *projection* we refer to a mapping from one alphabet to another. A projection $\alpha : \Gamma \to \Gamma'$ is lifted to pictures, words, picture languages, and word languages in the obvious way. For example, for every formula φ with free variables among $X_1, \ldots, X_t$, the picture language over $\{0,1\}^{t-1}$ defined by $\exists X_t \varphi$ is a projection of the picture language defined by φ, namely the image under the projection that maps $(b_1, \ldots, b_t)$ to $(b_1, \ldots, b_{t-1})$.

Since we want to use standard techniques from automata theory we pass from picture languages to word languages by fixing the height and considering columns of a picture as single symbols of a string.

Definition 7 *For a picture language L over alphabet Γ and an integer $m \geqslant 1$, we denote by $L(m)$ the following word language over $\Gamma^{m,1}$:*

$$L(m) = \left\{ \begin{pmatrix} a_{11} \\ \vdots \\ a_{m1} \end{pmatrix} \cdots \begin{pmatrix} a_{1n} \\ \vdots \\ a_{mn} \end{pmatrix} \middle| \begin{array}{ccc} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mn} \end{array} \in L \right\}$$

The next proposition provides the key argument against Σ_1-definability.

Proposition 8 *For every $t \geqslant 0$, and every formula $\varphi \in \Sigma_1$ with free variables among $X_1, \ldots, X_t$ there exists $c \geqslant 1$ such that for all $m \geqslant 1$ there is a nondeterministic finite automaton (NFA) with 2^{cm} states that recognizes the word language $Mod_t(\varphi)(m)$ over $(\{0,1\}^t)^{m,1}$.*

In Subsections 3.1 and 3.2 we will give two different proofs of Proposition 8. The second one uses the "standard" approach of Ehrenfeucht-Fraïssé games. The first one makes use of *tiling systems*, i.e., a notion of "recognizability" for picture languages, which (as shown in [GRST96]) coincides with Σ_1-definability.

Proposition 8 serves as induction base in the following theorem:

Theorem 9 *For every $k \geqslant 1$, $t \geqslant 0$, and every formula $\varphi \in \Sigma_k$ with free variables among $X_1, \ldots, X_t$ there exists $c \geqslant 1$ such that for all $m \geqslant 1$ there is an NFA with $s_k(cm)$ states that recognizes the word language $Mod_t(\varphi)(m)$ over $(\{0,1\}^t)^{m,1}$.*

For the proof we make use of the well-known constructions for complementation and projection of regular word languages: For every n-state NFA recognizing some word language L, there is (via the subset construction) a *deterministic* finite automaton (DFA) with 2^n states which recognizes L. Complementation of the set of accepting states then yields a DFA recognizing the complement of L. For an alphabet projection α, an n-state NFA for L can be turned into an n-state NFA for $\alpha(L)$: When reading some letter a, this NFA may go to any state to which the original automaton may go when reading some letter b with $\alpha(b) = a$.

Proof of Theorem 9. The proof is by induction on k. The case $k = 1$ is obtained from Proposition 8. For the induction step, assume we have proven the claimed implication for some k. Let φ be a Σ_{k+1}-formula with free variables among $X_1, \ldots, X_t$. W.l.o.g. we may assume that there is some $r \geqslant 0$ and a Σ_k-formula ψ with free variables among $X_1, \ldots, X_{t+r}$ such that $\varphi = \exists X_{t+1} \ldots \exists X_{t+r} \neg\psi$, i.e., $Mod_t(\varphi)$ is a projection of the complement of the picture language $Mod_{t+r}(\psi)$. So for every $m \geqslant 1$, the word language $Mod_t(\varphi)(m)$ is a projection of the complement of the word language $Mod_{t+r}(\psi)(m)$.

By induction hypothesis there is a $c \geqslant 1$ such that for every $m \geqslant 1$ there is an NFA with $s_k(cm)$ states that recognizes the word language $Mod_{t+r}(\psi)(m)$. Hence (by the above mentioned constructions for complementation and projection) the word language $Mod_t(\varphi)(m)$ is recognized by an NFA with $2^{s_k(cm)} = s_{k+1}(cm)$ states. □

We need some preparations on word languages over a singleton alphabet. For a one-letter alphabet a word is identified with its length and hence a word language is identified with a subset of $\mathbb{N}$. As in Definition 7, if $L \subseteq \mathbb{N} \times \mathbb{N}$ and $m \in \mathbb{N}$, we let $L(m) = \{n \in \mathbb{N} \mid (m, n) \in L\}$.

Definition 10 *Let $n \in \mathbb{N}$. A set N of integers is* periodic at n *(short: n-*periodic*) iff there is an integer $p \in \mathbb{N}$ such that $\forall l \geqslant n (l \in N \Leftrightarrow l + p \in N)$.*

Note that every boolean combination of n-periodic sets of integers is also n-periodic. (As period p take the least common multiple of the periods of the given sets.) It is well-known (see e.g. [Eil74]) that the regular languages over a one-letter alphabet are exactly those sets of integers that are n-periodic for some n.

The following Theorem of Chrobak ([Chr86]) states that any NFA with n states over a singleton alphabet can be transformed into an equivalent DFA whose transition structure is a loop together with a path of length at most $(n+2)^2$ from the initial state to this loop.

Theorem 11 ([Chr86], Theorem 4.4) *Let $N \subseteq \mathbb{N}$ be recognizable by some n-state NFA. Then there are some $k \leqslant (n+2)^2$ and an integer p such that N is recognized by a DFA $\mathcal{A}$ with states $0, \ldots, k + (p-1)$ such that $\mathcal{A}$ reaches the state $k + ((l-k) \mod p)$ after reading an input of length $l \geqslant k$.*

(In [Chr86], Chrobak states only that the above k can be chosen in $\mathcal{O}(n^2)$, which would also suffice for our purposes, but his proof shows the present stronger claim. Besides, he also gives an asymptotic bound for p, but we do not need that here.)

Corollary 12 *Let $N \subseteq \mathbb{N}$ be recognizable by some n-state NFA. Then N is $(n+2)^2$-periodic.*

Proof Let $\mathcal{A}$, k, p be as in the above theorem. For every $l \geqslant k$, the automaton reaches the same state on inputs of length either l or $l+p$. Thus $l \in N \iff l+p \in N$ for every $l \geqslant k$. $\square$

Now we apply Theorem 9 to sentences and hence to singleton alphabets.

Theorem 13 *Let $k \geqslant 1$ and φ be a $\mathrm{B}(\Sigma_k)$-sentence. There is a constant $c \geqslant 1$ such that for every $m \geqslant 1$ the set $Mod_0(\varphi)(m)$ is $s_k(cm)$-periodic.*

Proof Assume that φ is a boolean combination of the Σ_k-sentences $\varphi_1, \dots, \varphi_r$. By Theorem 9, there are $c_1, \dots, c_r$ such that for every $m \geqslant 1$ and every $i \leqslant r$, the set $Mod_0(\varphi_i)(m) = \{n \mid \underline{[m,n]} \models \varphi_i\}$ is recognized by some NFA with $s_k(c_i m)$ states. Let $c = \max\{4c_1, \dots, 4c_r\}$.
Since $(s_k(c_i m)+2)^2 \leqslant s_k(4c_i m) \leqslant s_k(cm)$ for every $m \geqslant 1$ and every $i \leqslant r$, Corollary 12 implies that $Mod_0(\varphi_i)(m)$ is $s_k(cm)$-periodic for every i. For every $m \geqslant 1$, the set $Mod_0(\varphi)(m)$ is a boolean combination of the sets $Mod_0(\varphi_1)(m), \dots, Mod_0(\varphi_r)(m)$ and hence also $s_k(cm)$-periodic. $\square$

Now we get Theorem 4, namely:

Corollary 14 *Every $\mathrm{B}(\Sigma_k)$-definable function is at most k-fold exponential.*

Proof Let f be definable by a $\mathrm{B}(\Sigma_k)$-sentence. By the above theorem, there is a c such that for all m, the singleton $\{f(m)\}$ is $s_k(cm)$-periodic. This implies that $f(m) \leqslant s_k(cm)$ for all m. $\square$

It remains to prove Proposition 8. The following two subsections provide two different proofs, which may be read independently. The first proof uses an automata theoretic approach involving the "tiling systems" of [GRST96] (which itself relies ultimately on Ehrenfeucht-Fraïssé games). For readers interested in a more self-contained exposition, we supply also a direct proof using Ehrenfeucht-Fraïssé games in Subsection 3.2.

3.1 Proving Proposition 8 via Tiling Systems

Definition 15 *Let P be a $m\times n$-picture over a finite alphabet Γ. We denote by $\hat{P}$ the $(m+2)\times(n+2)$-picture that results from P by surrounding it with the (fresh) boundary symbol $\#$.*

A local tiling system *over an alphabet Γ is a pair (Γ, Δ), where $\Delta \subseteq (\Gamma \cup \{\#\})^{2,2}$. The language recognized by a local tiling system $\mathcal{T} = (\Gamma, \Delta)$ is given by the set $\mathcal{L}(\mathcal{T})$ of pictures P such that all 2×2-subblocks of $\hat{P}$ are in Δ. A picture language $L \subseteq \Gamma^{+,+}$ is called* local *iff there is a local tiling system that recognizes L.*

In other words, a picture language is local iff membership of a picture P is completely determined by the set of $2{\times}2$-subblocks of $\hat{P}$. This generalizes the definition of "local word languages", where the membership of a word w is completely determined by the set of infixes of length 2 of $\#w\#$.

It is well-known that the regular word languages (which are the Σ_1-definable word languages) are projections of local word languages and conversely.

In the sequel we use such a representation of Σ_1-definable *picture* languages, as established in [GRST96]:

Theorem 16 ([GRST96], see also [GR96]) *A picture language is Σ_1-definable iff it is a projection of some local picture language.*

Proposition 17 *If L is a local picture language over alphabet Γ and $m \geqslant 1$, then $L(m)$ is a local word language over $\Gamma^{m,1}$.*

Proof Let (Γ, Δ) be a local tiling system recognizing L. Then a word w over $\Gamma^{m,1}$ is in $L(m)$ iff

all $2{\times}2$-subblocks of $\begin{array}{cc} \# & \# \\ \vdots & \overline{b} \\ \# & \# \end{array}$, (respectively of $\begin{array}{cc} \# & \# \\ \overline{a} & \overline{b} \\ \# & \# \end{array}$, respectively of $\begin{array}{cc} \# & \# \\ \overline{a} & \vdots \\ \# & \# \end{array}$)

are in Δ for the infix $\#\overline{b}$ of $\#w$ (respectively for all infixes $\overline{a}\,\overline{b}$ of w, respectively for the infix $\overline{a}\#$ of $w\#$), where $\overline{a}, \overline{b} \in \Gamma^{m,1}$. This means that $L(m)$ is a local word language. $\square$

As one can easily see, a local word language over an alphabet of size n is recognized by a deterministic finite automaton with $n + 1$ states.

Proof of Proposition 8. Let $t \geqslant 0$. From Theorem 16 we know that there exists a local tiling system $\mathcal{T} = (\Gamma, \Delta)$ and a projection $\alpha : \Gamma \to \{0,1\}^t$ such that $\alpha(\mathcal{L}(\mathcal{T})) = Mod_t(\varphi)$.

Let $d := |\Gamma| + 1$ and $c := \log_2 d$. For every $m \geqslant 1$, the word language $\mathcal{L}(\mathcal{T})(m)$ over alphabet $\Gamma^{m,1}$ is local and therefore recognized by some DFA with $|\Gamma^{m,1}| + 1 \leqslant d^m$ states. Since $\alpha(\mathcal{L}(\mathcal{T})(m)) = Mod_t(\varphi)(m)$ for every m, the above mentioned construction for projections of word languages gives, for every m, an NFA with $|\Gamma^{m,1}| + 1 \leqslant d^m = 2^{cm}$ states that recognizes $Mod_t(\varphi)(m)$. $\square$

3.2 Proving Proposition 8 via Ehrenfeucht-Fraïssé Games

Ehrenfeucht-Fraïssé games are played on two structures by two players, called *Spoiler* and *Duplicator*. Spoiler intends to show a difference between both structures while Duplicator tries to let them look alike. An introduction to Ehrenfeucht-Fraïssé games can be found in [EF95]. In order to prove

Proposition 8, we introduce the following kind of game. Let $q, t \geqslant 0$.

The q-round FO game on two t-bit grids R and R' of height m consists of q first-order rounds. In each round, Spoiler chooses a vertex in one of the two structures. Duplicator responds by choosing a vertex in the other structure.

Let x_j (resp. x'_j) be the vertex chosen in R (resp. in R') in the jth round. Duplicator wins iff the following three conditions are satisfied:

1. The mapping $x_j \mapsto x'_j$ (for all $j \leqslant q$) is a *partial isomorphism* between R and R'.

2. On the last 2^q columns Duplicator played *column-consistent*, i.e., if R is of width n and R' is of width n', and if, for each j, x_j is in column $n-\beta_j$ and x'_j is in column $n'-\beta'_j$, then $\beta_j < 2^q$ iff $\beta'_j < 2^q$, and if $\beta_j < 2^q$ then $\beta'_j = \beta_j$.

3. The last 2^q columns of R and R' are coloured identically, i.e., if $R = ([m, n], S_1, S_2, X_1, .., X_t)$ and $R' = ([m, n'], S'_1, S'_2, X'_1, .., X'_t)$, then for every $i \leqslant t$, $\alpha \leqslant m$, and $\beta \in \{0, .., 2^q-1\}$ we have $(\alpha, n-\beta) \in X_i$ iff $(\alpha, n'-\beta) \in X'_i$.

We write $R \cong_q R'$ iff Duplicator has a winning strategy in the q-round FO game on R and R'. Note that $\cong_q$ is an equivalence relation on the class of all t-bit grids. From the "easy part" of Ehrenfeucht's theorem (cf. [EF95], Theorem 1.2.8) one directly obtains the following (where FO^q denotes the class of all first-order formulas of quantifier depth at most q).

Lemma 18 *If $R \cong_q R'$, then, for all $\varphi \in \mathrm{FO}^q$, we have $R \models \varphi$ iff $R' \models \varphi$.*

Let R and P be two t-bit grids of equal height. With RP we denote the t-bit grid obtained by concatenating the leftmost column of P to the rightmost column of R. Winning conditions 2 and 3 are necessary to prove that $\cong_q$ is a congruence relation, i.e.:

Lemma 19 *For t-bit grids R, R', P of equal height, the following holds:*
If $R \cong_q R'$ then $RP \cong_q R'P$.

Proof Playing the q rounds according to Schwentick's Extension Theorem ([Sch96]), Duplicator directly obtains the following winning strategy on RP and $R'P$: Let $R = R_1R_2$ and $R' = R'_1R'_2$, where R_2 (and R'_2, respectively) consists of the last 2^q columns of R (and R', respectively). Winning condition 3 ensures that R_2 and R'_2 are coloured identically. Thus on R_2P, R'_2P Duplicator can win by simply choosing the same vertex as Spoiler did. On the other hand, on R_1R_2, $R'_1R'_2$ Duplicator can win according to her strategy on R, R', and winning condition 2 asserts that Duplicator can even play column-consistent on R_2, R'_2.

At the beginning of the game we view R_1 and R'_1 as the *strategy area*, P as the *identity area* and R_2 and R'_2 as the *buffer area*. Every time Spoiler chooses a vertex x in the *buffer area*, the three disjoint areas are modified: If x is closer to the *identity area* (with respect to the number of columns between x and this area), then the *identity area* is extended by all columns lying in the right-hand half of the *buffer area*. If x is closer to the *strategy area*, then the *strategy area* is extended by all columns lying in the left-hand half of the *buffer area*.

After this modification Spoiler's vertex lies either in the *strategy area* or in the *identity area*. In the *identity area* Duplicator responds with the identity, i.e. she chooses the vertex in the same row with the same distance from the rightmost column as Spoiler's vertex; in the *strategy area* Duplicator responds according to her strategy on R, R'.

After the pth round the width of the *buffer area* is at least 2^{q-p}. In particular, after q rounds no vertex chosen in the *strategy area* is adjacent to any vertex chosen in the *identity area*. Thus winning condition 1 is satisfied. As obviously winning conditions 2 and 3 are also satisfied, we have found a winning strategy for Duplicator in the q-round FO game on RP, $R'P$. $\square$

For a t-bit grid R, by $\langle R\rangle_{q,t}$ we denote the *equivalence class* of R, i.e., the set of all t-bit grids R' such that $R \cong_q R'$. With $e_{q,t}(m)$ we denote the number of equivalence classes in the q-round FO game on t-bit grids of height m. One can easily see that $e_{q,t}(m) \leqslant C \cdot 2^{t2^q m}$, where $2^{t2^q m}$ is the number of t-bit colourings of the last 2^q columns of a grid of height m, and C is a constant not depending on m (but only on t and q). Hence we obtain:

Lemma 20 *There is a $c_{q,t} \geqslant 1$ such that, for all m, $e_{q,t}(m) \leqslant 2^{c_{q,t}m}$.*

We can now use the Myhill-Nerode theorem (cf. [HU79], Theorem 3.9) to prove Proposition 8:

Proof of Proposition 8. Choose $r, q \geqslant 0$ such that $\varphi = \exists X_{t+1} \ldots \exists X_{t+r}\psi$, for some FO^q-formula ψ with free variables among $X_1, .., X_{t+r}$. Obviously, for every $m \geqslant 1$, the word language $Mod_t(\varphi)(m)$ is a projection of the word language $Mod_{t+r}(\psi)(m)$.

From the Myhill-Nerode theorem we know for every recognizable word language L that the number of states of the minimal DFA for L is exactly the number of equivalence classes (the *index*) of the Nerode congruence of L.[2] From the Lemmas 18 and 19 we conclude that the relation $\cong_q$ is finer than (and hence its index is larger than the index of) the Nerode congruence of $Mod_{t+r}(\psi)(m)$. Thus, for every m, there is a DFA for $Mod_{t+r}(\psi)(m)$ with $e_{q,t+r}(m) \leqslant 2^{cm}$ states, where $c := c_{q,t+r}$ is chosen according to Lemma 20.

[2] Two words u, v are Nerode-congruent w.r.t. L iff for all words w we have $uw \in L$ iff $vw \in L$.

The construction for projections of word languages gives an NFA with the same number of states, recognizing $Mod_t(\varphi)(m)$. $\square$

In particular, from the preceding proof one obtains that the constant c in Proposition 8 and Theorem 9 can be chosen depending only on the number of first-order and monadic second-order quantifiers of φ.

Let us mention that the above game-theoretical proof, and thus also Theorem 4, is still correct if the vertical order relation $\leqslant_1$ (but *not* both relations $\leqslant_1$ and $\leqslant_2$) is adjoined to the signature of grids.

4 How to Define k-fold Exponential Functions

In this section we show Theorem 5: We present, for each $k \geqslant 1$, a k-fold exponential function f_k such that the set of grids of size $(m, f_k(m))$ is Σ_k-definable (for short: such that f_k is Σ_k-definable). From Theorem 4 we know that f_k is *not* definable in $\mathrm{B}(\Sigma_{k-1})$ over τ_{Grid}.
Recall from Theorem 5 the definition of the functions f_k: $f_1(m) := 2^m$, $f_{k+1}(m) := f_k(m)2^{f_k(m)}$ for all $k, m \geqslant 1$. Speaking informally, our formula defining f_k describes a counting process on the underlying grid $\underline{[m,n]}$ which enforces n to be $f_k(m)$. This is achieved by labelling the grid with numbers in binary notation. Such a labelling is described by some subset of $[m,n]$ (containing the vertices with label 1). We proceed in two steps:

<u>**Step 1**</u>: As illustrated in Figure 1, starting with 0^m we write successive binary numbers of length m into the columns of the grid. n is a multiple of 2^m iff the rightmost column has number 1^m (and the numbering is called a *complete column-numbering*). In this case the grid can be divided into blocks of width $2^m = f_1(m)$, and the columns with number 0^m mark the starting points of these blocks.

<u>**Step $i{+}1$**</u> $(1{\leqslant}i{<}k)$: In the previous step the grid has been divided into blocks of width $f_i(m)$. As illustrated in Figure 2, starting with $0^{f_i(m)}$ we write successive binary numbers of length $f_i(m)$ into the top row of the grid. n is a multiple of $f_i(m)2^{f_i(m)} = f_{i+1}(m)$ iff the rightmost block has number $1^{f_i(m)}$ (and the numbering is called a *complete f_i-numbering*). In this case the grid can be divided into blocks of width $f_{i+1}(m)$, and the starting points of the subblocks with number $0^{f_i(m)}$ mark the starting points of these larger blocks.

Our formula defining the function f_k states that there exist sets $C, X_1, \ldots, X_k$, $Y_1, \ldots, Y_{k-1}$ such that C is a complete column-numbering, X_1 consists of the vertices marking the starting points of the blocks of width $f_1(m)$, for all $i < k$, Y_i is a complete f_i-numbering, X_{i+1} consists of the vertices marking the starting points of the blocks of width $f_{i+1}(m)$, and X_k consists of exactly one element.

$$\overbrace{\begin{array}{|c|c|c|c|c|}\hline 0&0&&1&1\\ \vdots&\vdots&\cdots&\vdots&\vdots\\ 0&0&&1&1\\ 0&1&&0&1\\ \hline\end{array}}^{f_1(m)=2^m}\!\!\begin{array}{|c|c|c|c|c|}\hline 0&0&&1&1\\ \vdots&\vdots&\cdots\quad\cdots&\vdots&\vdots\\ 0&0&&1&1\\ 0&1&&0&1\\ \hline\end{array}\!\!\begin{array}{|c|c|c|c|c|}\hline 0&0&&1&1\\ \vdots&\vdots&\cdots&\vdots&\vdots\\ 0&0&&1&1\\ 0&1&&0&1\\ \hline\end{array}\left.\vphantom{\begin{array}{c}0\\ \vdots\\ 0\\ 0\end{array}}\right\}m$$

Figure 1: The complete column-numbering of a grid.

$$\underbrace{\overbrace{\boxed{00\cdots00}}^{f_i(m)}\boxed{\cdots}\boxed{11\cdots11}}_{f_i(m)\cdot 2^{f_i(m)}=f_{i+1}(m)}\boxed{0\cdots\quad\cdots1}\boxed{00\cdots00}\boxed{\cdots}\boxed{11\cdots11}$$

Figure 2: The complete f_i-numbering of the top row of a grid.

4.1 Some helpful Remarks

Let $\mathcal{F}$ be a class of formulas. In this section, a formula φ (over the signature τ_{Grid}) is called an *$\mathcal{F}$-formula* if φ is equivalent (over the class of τ_{Grid}-structures) to a formula $\psi \in \mathcal{F}$ ($\varphi \equiv \psi$ for short).

Remark 21 *If $\varphi, \psi \in \Sigma_k$ (resp. Π_k), then for $* \in \{\wedge, \vee\}$ we have*

- $\varphi * \psi$ *is a Σ_k-formula (resp. a Π_k-formula),*
- $\neg\varphi$ *is a Π_k-formula (resp. a Σ_k-formula),*
- $\exists x\varphi$ *is a Σ_k-formula (resp. a Σ_{k+1}-formula),*
- $\forall x\varphi$ *is a Π_{k+1}-formula (resp. a Π_k-formula).*

Proof idea E.g. for the Σ_k-formula $\varphi := \exists X_1 \forall X_2 \cdots Q_k X_k\, \varphi'$, where $\varphi' \in$ FO, we have $\forall x\varphi \equiv \forall X \exists X_1 \forall X_2 \cdots Q_k X_k (\mathit{Singleton}(X) \rightarrow \forall x(Xx \rightarrow \varphi'))$, where $\mathit{Singleton}(X) := \exists x \forall y (Xy \leftrightarrow x = y)$ is a FO-formula asserting that X consists of exactly one element. $\square$

When interpreted over grids, the FO-formula $\mathit{left}(x) := \neg\exists y S_2 yx$ asserts that x is in the leftmost column of a grid. Let $\mathit{right}(x), \mathit{top}(x), \mathit{bottom}(x), \mathit{topleft}(x)$ etc. be similar formulas asserting that x is in the rightmost column, top row, bottom row, in the top left position, respectively.

For $x, y \in [m,n]$ let $\operatorname{int}(x,y] := \{\, y' \in [m,n] : x <_2 y' \leqslant_2 y \,\}$ and $\operatorname{int}(x,y) := \{\, y' \in [m,n] : x <_2 y' <_2 y \,\}$. Note that, in particular, $\operatorname{int}(x,y]$ and $\operatorname{int}(x,y)$ only contain vertices that are in the same row as x and y.
For $m, n \geqslant 1$, $x \in [m,n]$, and $X \subseteq [m,n]$, we denote by

$$\operatorname{Block}(X,x) \;:=\; \{\, y \in [m,n] : x \leqslant_2 y \text{ and } \operatorname{int}(x,y] \cap X = \emptyset \,\}$$

the set containing x and all vertices y to the right of x and in the same row as x, up to, but not including, the first vertex in X.
A vertex $y \in [m,n]$ is called *the X-successor of x* iff $x,y \in X$, $x <_2 y$, and $\mathrm{int}(x,y) \cap X = \emptyset$, i.e., $x,y \in X$ and for the vertex z such that S_2zy we have $z \in \mathrm{Block}(X,x)$.

Lemma 22 *There are Σ_1-formulas $Block(X,x,y)$ and $Succ(X,x,y)$ which express over grids that $y \in \mathrm{Block}(X,x)$, resp. that y is the X-successor of x.*

Proof The FO-formula $\varphi(B,X,x) :=$

$$\begin{array}{lll} \forall u & \{\, left(u) & \to \ (Bu \leftrightarrow u{=}x)\,\} \wedge \\ \forall u,v & \{\, S_2uv & \to \ (Bv \leftrightarrow (v{=}x \vee (Bu \wedge \neg Xv)))\,\} \end{array}$$

asserts that the set B consists of vertex x and all vertices to the right of x up to, but not including the first vertex in X. Thus the Σ_1-formula $Block(X,x,y) := \exists B(\varphi(B,X,x) \wedge By)$ asserts that $y \in \mathrm{Block}(X,x)$. Finally, define $Succ(X,x,y) := Xx \wedge Xy \wedge \exists z(S_2zy \wedge Block(X,x,z))$. $\square$

Let $X \subseteq [m,n]$. By $c_{m,n}(X)$ we denote the picture associated to the 1-bit grid $([m,n], S_1, S_2, X)$, i.e. $c_{m,n}(X) \in \{0,1\}^{m,n}$ is the picture of height m and width n which has 1's exactly at the positions in X.

4.2 How to describe the column-numbering

Definition 23 (column-numbering) *Let $m,n \geqslant 1$, $C \subseteq [m,n]$, and let $c_{i,j} := c_{m,n}(C)(i,j)$. For $j \leqslant n$ let $r_j < 2^m$ be the number represented by the binary string $c_{1,j} \cdots c_{m,j}$, standing in the jth column of $c_{m,n}(C)$, when read from the top to the bottom, i.e., $r_j := \sum_{i=1}^{m} c_{i,j} 2^{m-i} \in \{0,1,..,2^m-1\}$.*
We call C a column-numbering, *if and only if $r_1 = 0$ and $r_{j+1} \equiv r_j{+}1 \pmod{2^m}$ for all $j < n$; i.e., the leftmost column of $c_{m,n}(C)$ is 0^m and successive columns have successive C-numbers (modulo 2^m).*[3]

A column-numbering C is called complete *iff $r_n = 2^m{-}1$; i.e., the rightmost column of $c_{m,n}(C)$ is 1^m. (For an illustration see Figure 1.)*
Note that a complete column-numbering of $\underline{[m,n]}$ exists if and only if n is a multiple of 2^m.

The following easy proposition is useful for describing both the column-numbering and the f_k-numbering.

Proposition 24 *Let $q \geqslant 2$, $l \geqslant 1$. If $\overline{a} = a_1 \cdots a_l$ and $\overline{b} = b_1 \cdots b_l$, where $a_i, b_i \in \{0,..,q{-}1\}$, are the q-ary representations of length l of two natural numbers $a,b \in \{0,1,..,q^l{-}1\}$, i.e. $a = \sum_{i=1}^{l} a_i\, q^{l-i}$ and $b = \sum_{i=1}^{l} b_i\, q^{l-i}$, then we have $a{+}1 \equiv b \pmod{q^l}$ iff the following holds:*

[3]For integers r,s,t we write $r \equiv s \pmod{t}$ iff there is an integer k such that $r = kt{+}s$.

1. $a_l{+}1 \equiv b_l \pmod{q}$, *and*
2. *for all* $i > 1$*: If* $a_i = q{-}1$ *and* $b_i = 0$*,*
   then $a_{i-1}{+}1 \equiv b_{i-1} \pmod{q}$*, else* $a_{i-1} = b_{i-1}$*.*

Note that the condition "$a_i = q - 1$ *and* $b_i = 0$*" means that at position* $i{-}1$ *a carry of 1 must be added.*

Interpreting $\overline{a}$ and $\overline{b}$ as the C-colouring of two successive columns of a grid and applying Proposition 24 in the binary case (i.e. $q = 2$), we obtain the following lemma:

Lemma 25 (The column-numbering) *There are* FO*-formulas* $\mathit{col\text{-}num}(C)$ *and* $\mathit{compl\text{-}col\text{-}num}(C)$ *which express over grids that* C *is a column-numbering, resp. that* C *is a complete column-numbering.*

Proof Consider a grid $\underline{[m,n]}$. By Proposition 24 for $l := m$ and $q := 2$, we have:

For all $j \in \{1,..,n{-}1\}$: $r_{j+1} \equiv r_j{+}1 \pmod{2^m}$.

$\overset{\text{Prop. 24}}{\iff}$ For all $j \in \{1,..,n{-}1\}$:
- $c_{m,j}{+}1 \equiv c_{m,j+1} \pmod{2}$, and
- for all $i > 1$:
  if $c_{i,j} = 1$ and $c_{i,j+1} = 0$, then $c_{i-1,j} + 1 \equiv c_{i-1,j+1} \pmod{2}$,
  else $c_{i-1,j} = c_{i-1,j+1}$.

$\iff$
- For all $j \in \{1,..,n{-}1\}$: $(m,j) \in C \iff (m,j{+}1) \notin C$, and
- for all $j \in \{1,..,n{-}1\}$ and $i \in \{2,..,m\}$:
  if $x_0 := (i,j) \in C$ and $y_0 := (i,j{+}1) \notin C$,
  then $x_1 := (i{-}1,j) \in C \iff y_1 := (i{-}1,j{+}1) \notin C$
  else $x_1 \in C \iff y_1 \in C$.

This is expressed by the formula $\varphi(C) :=$

$$\begin{array}{rl} \forall x_0, y_0 & (\{\, \mathit{bottom}(x_0) \wedge S_2x_0y_0\} \rightarrow \{\, Cx_0 \leftrightarrow \neg Cy_0 \,\}) \wedge \\ \forall x_0, y_0, x_1, y_1 & (\{\, S_1x_1x_0 \wedge S_1y_1y_0 \wedge S_2x_0y_0 \,\} \rightarrow \\ & \{\, (\, (Cx_0 \wedge \neg Cy_0) \rightarrow (Cx_1 \leftrightarrow \neg Cy_1)) \wedge \\ & \;\; ((\neg(Cx_0 \wedge \neg Cy_0)) \rightarrow (Cx_1 \leftrightarrow Cy_1)) \quad \}). \end{array}$$

Hence, the formulas $\mathit{col\text{-}num}(C) := \varphi(C) \wedge \forall x\,(\mathit{left}(x) \rightarrow \neg Cx)$ and $\mathit{compl\text{-}col\text{-}num}(C) := \mathit{col\text{-}num}(C) \wedge \forall x\,(\mathit{right}(x) \rightarrow Cx)$ have the desired properties. □

Corollary 26 *The function* $f_1(m) := 2^m$ *is definable in* Σ_1 *and in* Π_1 *via the formulas*
$\sigma_1 := \exists C\{\mathit{compl\text{-}col\text{-}num}(C) \wedge \forall x, y((\mathit{top}(x) \wedge S_2xy \wedge Cx) \rightarrow Cy)\}$
and $\pi_1 := \forall C\,\{\, \mathit{col\text{-}num}(C) \rightarrow$
$[\forall x(\mathit{right}(x) \rightarrow Cx) \wedge \forall x, y((\mathit{top}(x) \wedge S_2xy \wedge Cx) \rightarrow Cy)]\,\}$.

4.3 How to describe the f_k-numbering

If $X \subseteq [m,n]$, $x = (i,j) \in [m,n]$ and $1 \leqslant l \leqslant (n-j+1)$, then we write $X(x,l)$ to denote the number represented by the binary string of length l which is in $c_{m,n}(X)$ on the l positions to the right of x (inclusively), i.e. $X(x,l) := \sum_{s=0}^{l-1} c_{m,n}(X)(i,j+s) \cdot 2^{l-1-s}$. (Note that we consider binary representations where the lowest bit is at the rightmost position.)

Definition 27 (f-marking, f-numbering)
Let $m,n \geqslant 1$, $X,Y \subseteq [m,n]$, and $f : \mathbb{N} \to \mathbb{N}$.

1. *We call X an* f-marking *iff X only contains top-row vertices and the top row of $c_{m,n}(X)$ is of the form $(10^{f(m)-1})^r$ for some $r \geqslant 1$; i.e., X divides the top row of $\underline{[m,n]}$ into blocks of width $f(m)$.*
   In particular, an f-marking of $\underline{\overline{[m,n]}}$ exists iff n is a multiple of $f(m)$.

2. *Let X be an f-marking. We call Y an* f-numbering *if and only if $Y((1,1),f(m)) = 0$ and $Y(y,f(m)) \equiv Y(x,f(m))+1 \pmod{2^{f(m)}}$ for all $x,y \in [m,n]$ such that y is the X-successor of x; i.e., in the top row of $c_{m,n}(Y)$ the leftmost block of width $f(m)$ is $0^{f(m)}$ and every two successive blocks of width $f(m)$ have successive Y-numbers.*

   An f-numbering Y is called complete, *iff $Y((1,n-f(m)+1),\, f(m)) = 2^{f(m)}-1$; i.e., in the top row of $c_{m,n}(Y)$ the rightmost block of width $f(m)$ is $1^{f(m)}$. (See Figure 2 for an illustration.)*
   Note that a complete f-numbering of $\underline{[m,n]}$ exists if and only if n is a multiple of $f(m)2^{f(m)}$.

The following Lemmas 28, 29, and 30 provide formulas which define f_k-markings, respectively f_k-numberings.

Lemma 28 (Describing the f_k-marking)

1. *There is a formula f_1-marking$(X,C) \in$ FO which expresses over grids that X is an f_1-marking, provided that C is a complete column-numbering.*

2. *There is a formula marking$(Z,X,Y) \in \Pi_1$ which expresses that Z is an f_{k+1}-marking, provided that X is an f_k-marking and Y a complete f_k-numbering.*

Proof ad 1. Let C be a complete column-numbering of $\underline{[m,n]}$ and let $r_j \in \{0,..,2^m-1\}$ be the C-number of the jth column. Then X is an f_1-marking iff X consists of all top-row vertices whose column-number is 0^m. To identify these columns, it suffices to look at the highest bits of the column-numbers: In column j the column-number switches from 1^m to 0^m iff the highest bit of the column-number switches from 1 to 0. Thus X is an f_1-marking iff $X = \{x = (1,j) \in [m,n] : j = 1 \text{ or } (x \notin C \text{ and } y = (1,j-1) \in C)\}$.

Hence, if C is a complete column-numbering, then the FO-formula

$$\begin{aligned} &f_1\text{-}marking(X, C) \ := \\ &\qquad \forall x\ (Xx\ \leftrightarrow\ (top(x)\ \wedge\ [topleft(x) \vee \exists y(S_2yx \wedge Cy \wedge \neg Cx)])\,) \end{aligned}$$

asserts that X is an f_1-marking.

ad 2. Let $k \geqslant 1$, and let X be an f_k-marking and Y a complete f_k-numbering. Then the top rows of $c_{m,n}(X)$ and $c_{m,n}(Y)$ are of the following form:

$$\begin{array}{r} c_{m,n}(X)\ : \\ c_{m,n}(Y)\ : \end{array} \ \underbrace{\left\| \begin{array}{c|c|c} \overbrace{\begin{array}{c} 10\cdots00 \\ 00\cdots00 \end{array}}^{f_k(m)} & \begin{array}{c} \cdots \\ \cdots \end{array} & \begin{array}{c} 10\cdots00 \\ 11\cdots11 \end{array} \end{array} \right\|}_{f_k(m)\cdot 2^{f_k(m)}\ =\ f_{k+1}(m)} \begin{array}{c} 1\cdots \quad \cdots 0 \\ 0\cdots \quad \cdots 1 \end{array} \underbrace{\left\| \begin{array}{c|c|c} 10\cdots00 & \cdots & 10\cdots00 \\ 00\cdots00 & \cdots & 11\cdots11 \end{array} \right\|}_{f_{k+1}(m)}$$

Obviously, Z is an f_{k+1}-marking if and only if Z consists of all vertices $x \in X$ for which the Y-number of $\mathrm{Block}(X, x)$ is $0^{f_k(m)}$, i.e. $Y(x, f_k(m)) = 0$. To identify these blocks it again suffices to look at the highest bits of the Y-numbers. Hence we obtain the correctness of the formula

$$\begin{array}{rrl} marking(Z, X, Y)\ := & \forall x & (\,Zx\ \rightarrow\ Xx\,)\ \wedge \\ & \forall x & (\,topleft(x)\ \rightarrow\ Zx\,)\ \wedge \\ & \forall x, y & (\,Succ(X, y, x)\ \rightarrow\ (Zx \leftrightarrow (Yy \wedge \neg Yx))\,). \end{array}$$

From Lemma 22 we know that $Succ(X, y, x) \in \Sigma_1$, and thus $marking(Z, X, Y)$ is a Π_1-formula (because "$Succ(X, y, x)\ \rightarrow\ \ldots$" is an abbreviation for "$\neg Succ(X, y, x) \vee \ldots$"). $\square$

Now we turn to the more difficult task of describing f_k-numberings (Lemmas 29 and 30). We start with some auxiliary formulas. Let $col\text{-}closed(X) := \forall x, x'(S_1xx' \rightarrow (Xx \leftrightarrow Xx'))$ be a FO-formula that expresses over grids that X is a union of columns; and let $row\text{-}closed(X)$ be a similar FO-formula expressing that X is a union of rows. The FO-formula $col(X, x) := col\text{-}closed(X) \wedge Xx \wedge \forall x', x''((Xx' \wedge top(x') \wedge Xx'' \wedge top(x'')) \rightarrow x'{=}x'')$ asserts that X consists exactly of all elements that are in the same row as x. Hence, the Σ_1-formula

$$\begin{aligned} &equal\text{-}col\text{-}num(C, x, y) \ := \\ &\quad \exists X, Y, Z\,\{\,col(X, x)\ \wedge\ col(Y, y)\ \wedge\ row\text{-}closed(Z) \wedge \\ &\qquad\qquad \forall z\,[(Xz \rightarrow (Zz \leftrightarrow Cz))\ \wedge\ (Yz \rightarrow (Zz \leftrightarrow Cz))]\,\} \end{aligned}$$

expresses over grids that the two columns of x and y have the same C-colouring. The Π_1-formulas

$$\begin{aligned} min(Y, x, X) \ &:= \ \forall z\,(Block(X, x, z) \rightarrow \neg Yz), \\ max(Y, x, X) \ &:= \ \forall z\,(Block(X, x, z) \rightarrow Yz) \end{aligned}$$

assert that $\mathrm{Block}(X, x) \cap Y = \emptyset$, resp. $\mathrm{Block}(X, x) \subseteq Y$, i.e. the Y-colouring of $\mathrm{Block}(X, x)$ consists of 0's, resp. 1's.

If X_k is an f_k-marking, then the Π_1-formulas[4]

$$\begin{array}{rcl} \mathit{leftmin}(Y, X_k) & := & \forall x \,(\, \mathit{topleft}(x) \rightarrow \mathit{min}(Y, x, X_k)\,),\\ \mathit{rightmax}(Y, X_k) & := & \forall x, y\; (\{\, \mathit{topright}(y) \;\wedge\; X_k x \;\wedge\; \mathit{Block}(X_k, x, y)\,\} \rightarrow \\ & & \{\, \mathit{max}(Y, x, X_k)\,\}) \end{array}$$

assert that $\mathrm{Block}(X_k, (1,1)) \cap Y = \emptyset$, resp. $\mathrm{Block}(X_k, (1, n - f_k(m) + 1)) \subseteq Y$, i.e. the leftmost (resp. rightmost) block of width $f_k(m)$ in the top row of $c_{m,n}(Y)$ consists of 0's (resp. 1's).
Table 1 contains a list of the most important formulas used in this section.

Name	Meaning (over grids)	Class
$\mathit{Block}(X, x, y)$	$y \in \mathrm{Block}(X, x)$	Σ_1
$\mathit{Succ}(X, x, y)$	y is the X-successor of x	Σ_1
$f_1\text{-}\mathit{marking}(X, C)$	X is an f_1-marking (if C is a complete column-numbering)	FO
$\mathit{marking}(Z, X, Y)$	Z is an f_{k+1}-marking (if X is an f_k-marking and Y a complete f_k-numbering)	Π_1
$(\mathit{compl}\text{-})\mathit{col}\text{-}\mathit{num}(C)$	C is a (complete) column-numbering	FO
$\mathit{equal}\text{-}\mathit{col}\text{-}\mathit{num}(C, x, y)$	the two columns of x and y have equal C-colouring	Σ_1
$\mathit{min}(Y, x, X)$	the Y-colouring of $\mathrm{Block}(X, x)$ consists of 0's	Π_1
$\mathit{max}(Y, x, X)$	the Y-colouring of $\mathrm{Block}(X, x)$ consists of 1's	Π_1
$\mathit{leftmin}(Y, X_k)$	the leftmost block of width $f_k(m)$ in the top row of $c_{m,n}(Y)$ consists of 0's (if X_k is an f_k-marking)	Π_1
$\mathit{rightmax}(Y, X_k)$	the rightmost block of width $f_k(m)$ in the top row of $c_{m,n}(Y)$ consists of 1's (if X_k is an f_k-marking)	Π_1
$\mathit{inc}_k(x, y, Y, C, \overline{X}_k, \overline{Y}_{k-1})$	the Y-number of $\mathrm{Block}(X_k, y)$ is one larger than the Y-number of $\mathrm{Block}(X_k, x)$ (if C is a complete column-numbering, X_i an f_i-marking for all $i \leqslant k$, Y_i a complete f_i-numbering for all $i < k$, and $x, y \in X_k$)	Π_k
$(\mathit{compl}\text{-})$ $f_k\text{-}\mathit{num}(Y, C, \overline{X}_k, \overline{Y}_{k-1})$	Y is a (complete) f_k-numbering (if C is a complete column-numbering, X_i an f_i-marking for all $i \leqslant k$, and Y_i a complete f_i-numbering for all $i < k$)	Π_k

Table 1: The most important formulas of Section 4.

An f_k-marking X_k divides the top row of a grid of height m into blocks of width $f_k(m)$. Of course, Y_k is a *complete f_k-numbering* iff the leftmost (resp. rightmost) block of width $f_k(m)$ entirely consists of zeroes (resp. ones) and every two successive blocks of width $f_k(m)$ have successive Y_k-numbers.

We compare the Y_k-numbers of two successive blocks of width $f_k(m)$ by comparing all corresponding subblocks of width $f_{k-1}(m)$. If Y_{k-1} is a complete f_{k-1}-numbering we can use the Y_{k-1}-number of a subblock as its address within the larger block. Applying Proposition 24, we obtain the

[4]Note that "$\mathit{topright}(y) \wedge X_k x \wedge \mathit{Block}(X_k, x, y)$" says that x is the starting point of the rightmost block of width $f_k(m)$ in the top row of a grid.

following:
The Y_k-number of a block B of width $f_k(m)$ is (modulo $2^{f_k(m)}$) one larger than the Y_k-number of a block A of width $f_k(m)$ iff the following holds:

1. The Y_k-number of the rightmost subblock in B is (modulo $2^{f_{k-1}(m)}$) one larger than the Y_k-number of the rightmost subblock in A, and

2. for every two successive subblocks B_1 and B_0 in B and A_1 and A_0 in A of width $f_{k-1}(m)$ such that B_0 and A_0 have the same Y_{k-1}-address, the following holds: If the Y_k-number of B_0 consists of zeroes (i.e., is equal to 0) and the Y_k-number of A_0 consists of ones (i.e., is equal to $2^{f_{k-1}(m)}-1$), *then* the Y_k-number of B_1 is (modulo $2^{f_{k-1}(m)}$) one larger than the Y_k-number of A_1 ; *else* B_1 and A_1 have equal Y_k-numbers.

A formalization of this condition inductively leads to a Π_k-formula asserting that two blocks of width $f_k(m)$ have successive Y_k-numbers. We shall write $\overline{X}_k$ as abbreviation for $X_1, .., X_k$ and $\overline{Y}_{k-1}$ as abbreviation for $Y_1, .., Y_{k-1}$.

Lemma 29 (How to compare f_k-numbers) *For all $k \geqslant 1$ there are Π_k-formulas $equal_k(x, y, Y, C, \overline{X}_k, \overline{Y}_{k-1})$ and $inc_k(x, y, Y, C, \overline{X}_k, \overline{Y}_{k-1})$ such that over grids the following holds: If C is a complete column-numbering, X_i an f_i-marking for all $i \leqslant k$, Y_i a complete f_i-numbering for all $i < k$, and $x, y \in X_k$, then*

1. *$equal_k(x, y, Y, C, \overline{X}_k, \overline{Y}_{k-1})$ expresses that* $\mathrm{Block}(X_k, x)$ *and* $\mathrm{Block}(X_k, y)$ *have the same Y-number, i.e., $Y(x, f_k(m)) = Y(y, f_k(m))$, and*
2. *$inc_k(x, y, Y, C, \overline{X}_k, \overline{Y}_{k-1})$ expresses that the Y-number of* $\mathrm{Block}(X_k, y)$ *is one larger than the Y-number of* $\mathrm{Block}(X_k, x)$, *i.e.,*
$Y(y, f_k(m)) \equiv Y(x, f_k(m)) + 1 \pmod{2^{f_k(m)}}$.

Proof We proceed by induction on k. $\underline{k = 1}$: Let X_1 be an f_1-marking of $[m, n]$, $x, y \in X_1$, and let C be a complete column-numbering, i.e.

		x								y					
$c_{m,n}(X_1)$:	$\cdots$	1	0	$\cdots$	0	0	1	$\cdots\cdots$	0	1	0	$\cdots$	0	0	1 $\cdots$
$c_{m,n}(Y)$:	$\cdots$	a_1	a_2	$\cdots$		a_l		$\cdots\cdots$		b_1	b_2	$\cdots$		b_l	$\cdots$
$c_{m,n}(C)$:	$\cdots$	$\begin{smallmatrix}0\\ \vdots\\ 0\\ 0\end{smallmatrix}$	$\begin{smallmatrix}0\\ \vdots\\ 0\\ 1\end{smallmatrix}$	$\cdots$	$\begin{smallmatrix}1\\ \vdots\\ 1\\ 0\end{smallmatrix}$	$\begin{smallmatrix}1\\ \vdots\\ 1\\ 1\end{smallmatrix}$	$\begin{smallmatrix}0\\ \vdots\\ 0\\ 0\end{smallmatrix}$	$\cdots\cdots$	$\begin{smallmatrix}1\\ \vdots\\ 1\\ 1\end{smallmatrix}$	$\begin{smallmatrix}0\\ \vdots\\ 0\\ 0\end{smallmatrix}$	$\begin{smallmatrix}0\\ \vdots\\ 0\\ 1\end{smallmatrix}$	$\cdots$	$\begin{smallmatrix}1\\ \vdots\\ 1\\ 0\end{smallmatrix}$	$\begin{smallmatrix}1\\ \vdots\\ 1\\ 1\end{smallmatrix}$	$\begin{smallmatrix}0\\ \vdots\\ 0\\ 0\end{smallmatrix}$ $\cdots$
		$\underbrace{\qquad\qquad}_{f_1(m)=2^m}$								$\underbrace{\qquad\qquad}_{f_1(m)=2^m}$					

where $l := 2^m$ and $a_1 \cdots a_l$ (resp. $b_1 \cdots b_l$) is the binary string standing in $c_{m,n}(Y)$ on the positions of $\mathrm{Block}(X_1, x)$ (resp. $\mathrm{Block}(X_1, y)$).
We compare two blocks of width 2^m bit by bit. Two positions in $\mathrm{Block}(X_1, x)$ and $\mathrm{Block}(X_1, y)$ denote corresponding bits iff they have the

same column-number. Hence we have $Y(x, 2^m) = Y(y, 2^m)$ if and only if the formula

$$\begin{array}{l} equal_1(x, y, Y, C, X_1) \ := \\ \quad \forall x_0, y_0 \ (\ \ \{ Block(X_1, x, x_0) \ \wedge \ Block(X_1, y, y_0) \ \wedge \\ \qquad\qquad\qquad equal\text{-}col\text{-}num(C, x_0, y_0) \ \} \ \rightarrow \\ \qquad\qquad\quad \{ Yx_0 \ \leftrightarrow \ Yy_0 \} \ ) \end{array}$$

is satisfied in $\underline{[m,n]}$.

In the way explained before Lemma 29, as an application of Proposition 24 (for $l = 2^m$, $q = 2$) we obtain that $Y(x, 2^m){+}1 \ \equiv \ Y(y, 2^m) \pmod{2^l}$ iff the following formula[5] is true in $\underline{[m,n]}$:

$$\begin{array}{lll} inc_1(x, y, Y, C, X_1) \ := & & \\ \quad \forall x_0, y_0 & (& \{ Block(X_1, x, x_0) \ \wedge \ (right(x_0) \ \vee \ \exists z(S_2 x_0 z \wedge X_1 z)) \ \wedge \\ & & \ \ Block(X_1, y, y_0) \ \wedge \ (\, right(y_0) \ \vee \ \exists z(S_2 y_0 z \wedge X_1 z)) \quad \} \ \rightarrow \\ & & \{ Yx_0 \ \leftrightarrow \ \neg Yy_0 \} \ ) \ \wedge \\ \forall x_1, x_0, y_1, y_0 & (& \{ Block(X_1, x, x_1) \ \wedge \ Block(X_1, x, x_0) \ \wedge \ S_2 x_1 x_0 \ \wedge \\ & & \ \ Block(X_1, y, y_1) \ \wedge \ Block(X_1, y, y_0) \ \wedge \ S_2 y_1 y_0 \ \wedge \\ & & \ \ equal\text{-}col\text{-}num(C, x_0, y_0) \} \ \ \rightarrow \\ & & \{ (\ \ (Yx_0 \ \wedge \ \neg Yy_0) \ \ \rightarrow \ (Yx_1 \leftrightarrow \neg Yy_1) \,) \ \wedge \\ & & \ \ ((\neg (Yx_0 \wedge \neg Yy_0)) \ \rightarrow \ (Yx_1 \leftrightarrow Yy_1) \,) \ \ \} \,) \, . \end{array}$$

As $Block(X_1, x, x_0)$ and $equal\text{-}col\text{-}num(C, x_0, y_0)$ are in Σ_1, $inc_1(x, y, Y, C, X_1)$ and $equal_1(x, y, Y, C, X_1)$ are Π_1-formulas.

$\underline{k \mapsto k{+}1}$: Let X_{k+1} be an f_{k+1}-marking, $x, y \in X_{k+1}$, and X_i an f_i-marking and Y_i a complete f_i-numbering for all $i \leqslant k$. I.e., the top rows of $c_{m,n}(X_{k+1})$, $c_{m,n}(Y)$, $c_{m,n}(X_k)$, and $c_{m,n}(Y_k)$ are of the following form:

$$\begin{array}{rcl} & & \qquad\qquad x \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad y \\ c_{m,n}(X_{k+1}) & : & \cdots \| \ 10\cdots00 \ \ \cdots \ \ 00\cdots00 \ \| \cdots\cdot \| \ 10\cdots00 \ \ \cdots \ \ 00\cdots00 \ \| \cdots \\ c_{m,n}(Y) & : & \cdots \| \quad \overline{a}_1 \quad | \cdots | \quad \overline{a}_l \quad \| \cdots\cdot \| \quad \overline{b}_1 \quad | \cdots | \quad \overline{b}_l \quad \| \cdots \\ c_{m,n}(X_k) & : & \cdots \| \ 10\cdots00 \ | \cdots | \ 10\cdots00 \ \| \cdots\cdot \| \ 10\cdots00 \ | \cdots | \ 10\cdots00 \ \| \cdots \\ c_{m,n}(Y_k) & : & \cdots \| \ 00\cdots00 \ | \cdots | \ 11\cdots11 \ \| \cdots\cdot \| \ 00\cdots00 \ | \cdots | \ 11\cdots11 \ \| \cdots \\ & & \qquad \underbrace{\qquad\qquad\qquad\qquad\qquad}_{f_k(m)\cdot 2^{f_k(m)} \ = \ f_{k+1}(m)} \qquad \underbrace{\qquad\qquad\qquad\qquad\qquad}_{f_k(m)\cdot 2^{f_k(m)} \ = \ f_{k+1}(m)} \end{array}$$

where $l = 2^{f_k(m)}$, and $\overline{a}_i, \overline{b}_i \in \{0,1\}^{f_k(m)}$ (for $i \in \{1, .., l\}$) such that $\overline{a}_1 \overline{a}_2 \cdots \overline{a}_l$ (resp. $\overline{b}_1 \overline{b}_2 \cdots \overline{b}_l$) is the binary string standing in $c_{m,n}(Y)$ on the positions of $\mathrm{Block}(X_{k+1}, x)$ (resp. $\mathrm{Block}(X_{k+1}, y)$).

We compare the Y-colouring of two blocks of width $f_{k+1}(m)$ by comparing all corresponding subblocks of width $f_k(m)$. As Y_k is a complete f_k-numbering, we can use the Y_k-number of a subblock as its address within the block. We use the formula $equal_k$ both to compare addresses and to compare Y-colourings of subblocks of width $f_k(m)$.

[5]Note that "$Block(X_1, x, x_0) \ \wedge \ (right(x_0) \ \vee \ \exists z(S_2 x_0 z \wedge X_1 z))$" asserts that x_0 is on the rightmost position of $\mathrm{Block}(X_1, x)$.

Hence we express $Y(x, f_{k+1}(m)) = Y(y, f_{k+1}(m))$ by the formula

$$
\begin{aligned}
&\mathit{equal}_{k+1}(x, y, Y, C, \overline{X}_{k+1}, \overline{Y}_k) \ := \\
&\quad \forall\, x_0, y_0 \quad (\ \{ \mathit{Block}(X_{k+1}, x, x_0) \ \wedge \ X_k x_0 \ \wedge \\
&\qquad\qquad \mathit{Block}(X_{k+1}, y, y_0) \ \wedge \ X_k y_0 \ \wedge \\
&\qquad\qquad \mathit{equal}_k(x_0, y_0, Y_k, C, \overline{X}_k, \overline{Y}_{k-1}) \ \} \rightarrow \\
&\qquad\qquad \mathit{equal}_k(x_0, y_0, Y, C, \overline{X}_k, \overline{Y}_{k-1}) \ ) \, .
\end{aligned}
$$

By induction we have $\mathit{equal}_k \in \Pi_k$, and thus equal_{k+1} is a Π_{k+1}-formula.

In the way explained before Lemma 29, as an application of Proposition 24 (for $q = l = 2^{f_k(m)}$) we obtain that $Y(x, f_{k+1}(m)){+}1 \equiv Y(y, f_{k+1}(m)) \pmod{2^l}$ is expressed by

$$
\begin{aligned}
&\mathit{inc}_{k+1}(x, y, Y, C, \overline{X}_{k+1}, \overline{Y}_k) \ := \\
&\quad \forall\, x_0, y_0 \qquad (\ \{ \mathit{Block}(X_{k+1}, x, x_0) \wedge X_k x_0 \ \wedge \ \mathit{max}(Y_k, x_0, X_k) \wedge \\
&\qquad\qquad \mathit{Block}(X_{k+1}, y, y_0) \ \wedge X_k y_0 \ \wedge \ \mathit{max}(Y_k, y_0, X_k) \ \} \rightarrow \\
&\qquad\qquad \mathit{inc}_k(x_0, y_0, Y, C, \overline{X}_k, \overline{Y}_{k-1}) \ ) \ \wedge \\
&\quad \forall\, x_1, x_0, y_1, y_0 \quad (\\
&\qquad \{ \ \mathit{Block}(X_{k+1}, x, x_1) \wedge \mathit{Block}(X_{k+1}, x, x_0) \wedge \mathit{Succ}(X_k, x_1, x_0) \wedge \\
&\qquad\ \ \mathit{Block}(X_{k+1}, y, y_1) \ \wedge \mathit{Block}(X_{k+1}, y, y_0) \ \wedge \mathit{Succ}(X_k, y_1, y_0) \ \wedge \\
&\qquad\ \ \mathit{equal}_k(x_0, y_0, Y_k, C, \overline{X}_k, \overline{Y}_{k-1}) \ \} \ \rightarrow \\
&\qquad \{ \ [\quad (\mathit{max}(Y, x_0, X_k) \wedge \mathit{min}(Y, y_0, X_k)) \ \rightarrow \ \mathit{inc}_k(x_1, y_1, Y, C, \overline{X}_k, \overline{Y}_{k-1}) \,] \ \wedge \\
&\qquad\ \ [\, (\neg(\mathit{max}(Y, x_0, X_k) \wedge \mathit{min}(Y, y_0, X_k))) \ \rightarrow \mathit{equal}_k(x_1, y_1, Y, C, \overline{X}_k, \overline{Y}_{k-1}) \,] \, \}) \, .
\end{aligned}
$$

Here, $\mathit{max}(Y, x, X)$ and $\mathit{min}(Y, x, X)$ are the Π_1-formulas as defined before, asserting that $\mathrm{Block}(X, x) \subseteq Y$ and $\mathrm{Block}(X, x) \cap Y = \emptyset$, respectively. By induction we have $\mathit{inc}_k, \mathit{equal}_k \in \Pi_k$. Hence inc_{k+1} is a Π_{k+1}-formula.
$\square$

Using the Π_k-formula inc_k, we can now construct a Π_k-formula asserting that Y is a (complete) f_k-numbering:

Lemma 30 (Describing the f_k-numbering) *For all $k \geqslant 1$ there are Π_k-formulas f_k-$\mathit{num}(Y, C, \overline{X}_k, \overline{Y}_{k-1})$ and compl-f_k-$\mathit{num}(Y, C, \overline{X}_k, \overline{Y}_{k-1})$ such that over grids the following holds: If C is a complete column-numbering, X_i an f_i-marking for all $i \leqslant k$, and Y_i a complete f_i-numbering for all $i < k$, then f_k-$\mathit{num}(Y, C, \overline{X}_k, \overline{Y}_{k-1})$ expresses that Y is an f_k-numbering, and compl-f_k-$\mathit{num}(Y, C, \overline{X}_k, \overline{Y}_{k-1})$ expresses that Y is a complete f_k-numbering.*

Proof Let $\mathit{leftmin}(Y, X_k)$ and $\mathit{rightmax}(Y, X_k)$ be the Π_1-formulas as defined before. Y is an f_k-numbering of $\underline{[m, n]}$ iff $Y((1,1), f_k(m)) = 0$ and for all $x, y \in [m, n]$ such that y is the X_k-successor of x, we have $Y(y, f_k(m)) \equiv Y(x, f_k(m)){+}1 \pmod{2^{f_k(m)}}$. Hence, from Lemma 29 we conclude that the Π_k-formula f_k-$\mathit{num}(Y, C, \overline{X}_k, \overline{Y}_{k-1}) :=$

$$\mathit{leftmin}(Y, X_k) \ \wedge \ \forall x, y \, (\mathit{Succ}(X_k, x, y) \rightarrow \mathit{inc}_k(x, y, Y, C, \overline{X}_k, \overline{Y}_{k-1}))$$

asserts that Y is an f_k-numbering. To assert that Y is a complete f_k-numbering, a formula additionally has to express that the rightmost block of width $f_k(m)$ of the top row of $c_{m,n}(Y)$ consists of 1's. This is expressed by the Π_k-formula $\mathit{compl}\text{-}f_k\text{-}\mathit{num}(Y, C, \overline{X}_k, \overline{Y}_{k-1}) :=$

$$f_k\text{-}\mathit{num}(Y, C, \overline{X}_k, \overline{Y}_{k-1}) \ \wedge\ \mathit{rightmax}(Y, X_k) \qquad \square$$

4.4 Proof of Theorem 5

Applying the preceding lemmas, we can now present a Σ_k-formula σ_k and a Π_k-formula π_k such that $\mathit{Mod}_{\mathrm{Grid}}(\sigma_k) = \mathit{Mod}_{\mathrm{Grid}}(\pi_k) = \{\underline{[m, f_k(m)]} : m \geqslant 1\}$, and thus prove part 1 of Theorem 5.

Proof of Part 1 of Theorem 5: Σ_k- and Π_k-Definability of f_k.

We define $\sigma_k :=$

$$\begin{aligned} &\exists\, C, X_1, .., X_k, Y_1, .., Y_{k-1}\ \{\\ &\qquad \mathit{compl}\text{-}\mathit{col}\text{-}\mathit{num}(C)\ \wedge\ f_1\text{-}\mathit{marking}(X_1, C)\ \wedge\\ &\qquad \textstyle\bigwedge_{i=1}^{k-1}\ (\ \mathit{compl}\text{-}f_i\text{-}\mathit{num}(Y_i, C, \overline{X}_i, \overline{Y}_{i-1})\ \wedge\ \mathit{marking}(X_{i+1}, X_i, Y_i)\ )\ \wedge\\ &\qquad \mathit{Singleton}(X_k)\ \}\,, \end{aligned}$$

where $\mathit{Singleton}(X_k) := \exists x \forall y (X_k y \leftrightarrow x = y)$ is a FO-formula asserting that X_k consists of exactly one element.

From the Lemmas 25, 28 and 30 we conclude for all $m, n \geqslant 1$ that[6] $\underline{[m,n]} \models \sigma_k$ iff $n = f_k(m)$. As $f_1\text{-}\mathit{marking} \in$ FO, $\mathit{marking} \in \Pi_1$, $\mathit{compl}\text{-}\mathit{col}\text{-}\mathit{num} \in$ FO, and $\mathit{compl}\text{-}f_j\text{-}\mathit{num} \in \Pi_j$ for all $j \geqslant 1$, we obtain that σ_k is a Σ_k-formula.

To obtain a Π_k-formula which defines f_k, we show that the set $\{\underline{[m,n]} : n \neq f_k(m)\}$ can be defined by a Σ_k-formula ϱ_k.

For integers r and s we write $r \mid s$ if s is a multiple of r, and $r \nmid s$ otherwise. Obviously the following holds:

$$\begin{array}{lllll} n \neq f_k(m) \iff & (\, f_1(m) \nmid n\,) & \text{or} & & \\ & (\, f_1(m) \mid n & \text{and} & f_2(m) \nmid n\,) & \text{or} \\ & \quad\vdots & \quad\vdots & \quad\vdots & \vdots \\ & (\, f_{k-1}(m) \mid n & \text{and} & f_k(m) \nmid n\,) & \text{or} \\ & (\, f_k(m) \mid n & \text{and} & n \neq f_k(m)\,)\,. & \end{array}$$

Of course, we have $f_1(m) \nmid n$ iff there is a column-numbering C such that the rightmost column of $c_{m,n}(C)$ does not entirely consist of 1's.

This property is asserted by the Σ_1-formula

$$\varphi_0 := \exists\, C\, \{\mathit{col}\text{-}\mathit{num}(C)\ \wedge\ \exists x\, (\mathit{right}(x) \wedge \neg C x)\}.$$

For $j \in \{1, .., k-1\}$ we have $f_j(m) \mid n$ and $f_{j+1}(m) \nmid n$ iff there is an f_j-marking, but there is no complete f_j-numbering. Obviously, this is

[6] Note that σ_k indeed describes the counting process explained at the beginning of Section 4.

expressed by the Σ_{j+1}-formula

$$\begin{aligned}\varphi_j \ :=\ \exists\, C, X_1, .., X_j, Y_1, .., Y_j\ \{ & \\ & compl\text{-}col\text{-}num(C)\ \wedge\ f_1\text{-}marking(X_1,C)\ \wedge \\ & \textstyle\bigwedge_{i=1}^{j-1}\ (\ compl\text{-}f_i\text{-}num(Y_i, C, \overline{X}_i, \overline{Y}_{i-1})\ \wedge\ marking(X_{i+1}, X_i, Y_i)\ )\ \wedge \\ & f_j\text{-}num(Y_j, C, \overline{X}_j, \overline{Y}_{j-1})\ \wedge\ \neg rightmax(Y_j, X_j)\,\}.\end{aligned}$$

Furthermore, we have $f_k(m) \mid n$ and $n \neq f_k(m)$ iff there is an f_k-marking X_k and $|X_k| \neq 1$. This is asserted by the Σ_k-formula

$$\begin{aligned}\varphi_k \ :=\ \exists\, C, X_1, .., X_k, Y_1, .., Y_{k-1}\ \{ & \\ & compl\text{-}col\text{-}num(C)\ \wedge\ f_1\text{-}marking(X_1,C)\ \wedge \\ & \textstyle\bigwedge_{i=1}^{k-1}\ (\ compl\text{-}f_i\text{-}num(Y_i, C, \overline{X}_i, \overline{Y}_{i-1})\ \wedge\ marking(X_{i+1}, X_i, Y_i)\ )\ \wedge \\ & \neg Singleton(X_k)\,\}.\end{aligned}$$

We hence obtain $n \neq f_k(m)$ iff $\underline{[m,n]}$ satisfies $\varrho_k := \bigvee_{j=0}^{k} \varphi_j$, where $\varrho_k \in \Sigma_k$. Thus, $\pi_k := \neg\varrho_k$ is a Π_k-formula which defines f_k. □

Proof of Part 2 of Theorem 5: Σ_1- and Π_1-Definability of f_k over $\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\}$.

In the context of formulas over the signature $\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\}$, a grid $\underline{[m,n]}$ is always identified with the structure $([m,n], S_1, S_2, \leqslant_1, \leqslant_2)$, where the binary predicate $\leqslant_i$ is interpreted as the transitive closure of S_i for $i \in \{1,2\}$.

We will now show that for each $k \geqslant 1$ the k-fold exponential function f_k is definable in Σ_1 and in Π_1 over $\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\}$, i.e. there are formulas $\sigma_k \in \Sigma_1$ and $\pi_k \in \Pi_1$ over the signature $\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\}$ such that $Mod_{\text{Grid}}(\sigma_k) = Mod_{\text{Grid}}(\pi_k) = \{([m, f_k(m)], S_1, S_2, \leqslant_1, \leqslant_2) \,:\, m \geqslant 1\}$.

We have a closer look at the formulas developed in the previous subsections. In Lemma 22 we have constructed a Σ_1-formula $Block(X,x,y)$ asserting that $y \in \text{Block}(X,x)$. Over grids with built-in horizontal order $\leqslant_2$, we can do this in first-order logic via the formula

$$Block(X,x,y) \ :=\ x \leqslant_2 y\ \wedge\ \forall y'\{(\neg y'{=}x\ \wedge\ x \leqslant_2 y'\ \wedge\ y' \leqslant_2 y) \rightarrow \neg Xy'\}.$$

From this, we obtain a FO-formula

$$Succ(X,x,y) \ :=\ Xx\ \wedge\ Xy\ \wedge\ \exists z(S_2 zy \wedge Block(X,x,z))$$

asserting that y is the X-successor of x.

Furthermore, using the order relations $\leqslant_1$ and $\leqslant_2$, we can construct a FO-formula $equal\text{-}col\text{-}num(C,x,y)$ asserting that x and y lie in columns of equal C-number: The FO-formula "$row(u,v) := u{\leqslant_2}v\ \vee\ v{\leqslant_2}u$" expresses that u and v lie in the same row of a grid. Analogously we obtain a formula $col(u,v)$ asserting that u and v are in the same column of a grid. Hence, the FO-formula

$$\begin{aligned}& equal\text{-}col\text{-}num(C,x,y) \ := \\ & \qquad \forall x_0, y_0\, \{(col(x_0,x)\ \wedge\ col(y_0,y)\ \wedge\ row(x_0,y_0))\ \rightarrow\ (Cx_0 \leftrightarrow Cy_0)\}\end{aligned}$$

expresses that x and y are in columns of equal C-number.

Using the FO-formulas *Block*, *Succ*, and *equal-col-num* in the Lemmas 28, 29, and 30, we obtain FO-formulas over the signature $\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\}$ such that the formulas σ_k and π_k from the proof of part 1 of Theorem 5 now are in Σ_1 and in Π_1, respectively. $\square$

In particular, we conclude that over grids with built-in vertical and horizontal order-relations, Theorem 4 is *not* valid, i.e. we do not obtain an upper bound on the growth rate of $\mathrm{B}(\Sigma_k)$-definable functions.

Proof of Parts 3 and 4 of Theorem 5.

Parts 3 and 4 of Theorem 5 say that f_k is definable in $\Sigma_1^{\text{TC}(1)}$ and in $\Pi_1^{\text{TC}(1)}$ over τ_{Grid}, as well as by a sentence of the form $\exists\overline{X}\psi$ with $\psi \in \mathrm{PFO}(\Sigma_1)$ and by a sentence of the form $\forall\overline{X}\psi'$, where $\psi' \in \mathrm{PFO}(\Pi_1)$. For the proof we will apply part 2 of Theorem 5 together with the following lemma.

Lemma 31 *For $i \in \{1, 2\}$, the atomic $\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\}$-formula $x \leqslant_i y$ is equivalent over grids to a $\mathrm{FO}^{\text{TC}(1)}$-formula, to a Π_1-formula, and to a Σ_1-formula over τ_{Grid}.*

Proof The formula $x \leqslant_i y$ is equivalent to the $\mathrm{FO}^{\text{TC}(1)}$-formula $\mathrm{TC}(x, y, S_i xy)(x, y)$.
Secondly, $x \leqslant_i y$ is equivalent to a Π_1-formula which says that every set X which contains x and is closed under S_i-successors also contains y.
Finally, $x \leqslant_i y$ is equivalent to a Σ_1-formula which says that there is a set X such that x is the only element of X which has no S_i-predecessor in X and y is the only element of X that has no S_i-successor in X. $\square$

From part 2 of Theorem 5 we obtain formulas $\sigma_k \in \Sigma_1$ and $\pi_k \in \Pi_1$ over $\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\}$ which define the function f_k.
By replacing every atomic formula $x \leqslant_i y$ in σ_k and in π_k by the $\mathrm{FO}^{\text{TC}(1)}$-formula from Lemma 31, we obtain formulas in $\Sigma_1^{\text{TC}(1)}$ and in $\Pi_1^{\text{TC}(1)}$ over τ_{Grid} which define f_k.

To prove claim 4, we assume that σ_k is of the form $\exists\overline{X}\,\xi_1 x_1 \ldots \xi_r x_r\,\varphi$, where $\overline{X}$ is a tuple of monadic second-order variables, $\xi_i \in \{\exists, \forall\}$ for all $i \leqslant r$, and φ is a conjunction of disjunctions of negated or unnegated atomic $(\tau_{\text{Grid}} \cup \{\leqslant_1, \leqslant_2\})$-formulas. Replacing every unnegated (resp. negated) occurrence of "$x \leqslant_i y$" by the Σ_1-formula (resp. by the Π_1-formula) from Lemma 31, we obtain from φ a Σ_1-formula σ over τ_{Grid} such that the formula $\exists\overline{X}\,\xi_1 x_1 \ldots \xi_r x_r\,\sigma$ defines the function f_k. Analogously, from π_k we obtain a formula $\forall\overline{X}\,\xi_1 x_1 \ldots \xi_r x_r\,\sigma'$, where $\sigma' \in \Pi_1$. $\square$

5 From Grids to Graphs

Now we show how to transfer separation results from one class $\mathcal{C}$ of structures to a different class $\mathcal{C}'$, possibly over a different signature. Basically, a $\mathcal{C}$-structure has to be encoded in a $\mathcal{C}'$-structure in such a way that any formula talking about a $\mathcal{C}$-structure M can be transformed into a formula that says the same about the encoding of M and, conversely, every formula talking about a $\mathcal{C}'$-structure M' can be transformed into a formula that says the same about the $\mathcal{C}$-structure whose encoding M' is, if such a structure exists. Moreover, the translation of formulas has to respect the formula classes under consideration.

We apply this technique to transfer the non-inclusion results obtained in the previous sections from grids to directed graphs and from directed to undirected graphs.

5.1 Strong First-Order Reductions

We introduce the notion of "strong first-order reducibility" as a tool to transfer separation results from one class of structures to another. Here we consider the more general case of arbitrary relational signatures (instead of just τ_{Grid}, τ_{Graph}).

Strong first-order reductions are a version of interpretations (see e.g. [Rab77, Hog93]), more precisely a refinement of "monadic first-order reductions" as defined in [Cos93]. It is a certain kind of function that codes a structure M over some signature τ into another structure $\Phi(M)$ over a possibly different signature τ' in such a way that a formula φ over signature τ can be translated into a formula φ' over τ' (and vice versa) such that φ and φ' are on the same level of the alternation hierarchy and φ' asserts for $\Phi(M)$ the same as φ asserts for M. The domain of $\Phi(M)$ will be of the form $\{1, \dots, n\} \times \text{dom}(M)$.

Definition 32 *Let $\mathcal{C}$, $\mathcal{C}'$ be classes of structures over the relational signatures τ and τ', respectively. Let $n \geqslant 1$.*

A strong first-order reduction from $\mathcal{C}$ to $\mathcal{C}'$ with rank n *is an injective mapping $\Phi : \mathcal{C} \to \mathcal{C}'$ such that*

1. *For every structure $M \in \mathcal{C}$ the universe of $\Phi(M)$ is given by $\bigcup_{i \leqslant n}(\{i\} \times \text{dom}M)$, i.e., a disjoint union of n copies of the universe of M.*

2. *There is a first-order formula $\psi(x_1, \dots, x_n)$ over τ' such that for all structures M in $\mathcal{C}$, all $u_1, \dots, u_n \in \text{dom}M$, and all $i_1, \dots, i_n \leqslant n$:*

$$\Phi(M) \models \psi[(i_1, u_1), \dots, (i_n, u_n)] \quad \textit{iff} \quad \forall j \leqslant n : i_j = j \wedge u_j = u_1.$$

(For structures in $\Phi(\mathcal{C})$, the formula ψ describes the n-tuples of the form $((1, u), \dots, (n, u))$, which serve as representations of M-elements u.)

3. *For every relation symbol r' from τ', say of arity l, and every $\kappa : [l] \to [n]$ there is an* FO*-formula $\varphi_\kappa^{r'}(x_1, \ldots, x_l)$ over τ such that for all structures M in $\mathcal{C}$ and all $u_1, \ldots, u_l \in \mathrm{dom} M$ we have*

$$M \models \varphi_\kappa^{r'}[u_1, \ldots, u_l] \quad \textit{iff} \quad \Phi(M) \models r'[(\kappa(1), u_1), \ldots, (\kappa(l), u_l)].$$

4. *For every relation symbol r from τ, say of arity l, there is a first-order formula $\varphi^r(x_1, \ldots, x_l)$ over τ' such that for all structures M in $\mathcal{C}$ and all $u_1, \ldots, u_l \in \mathrm{dom} M$ we have*

$$M \models r[u_1, \ldots, u_l] \quad \textit{iff} \quad \Phi(M) \models \varphi^r[(1, u_1), \ldots, (1, u_l)].$$

$\mathcal{C}$ is strongly first-order reducible *to $\mathcal{C}'$ iff there is a strong first-order reduction from $\mathcal{C}$ to $\mathcal{C}'$.*

Strong first-order reducibility is transitive and reflexive, but we do not claim that it is symmetric. In Proposition 38 we give three examples for strong first-order reductions.

We wish to show the following:

Theorem 33 *Let $\mathcal{C}$, $\mathcal{C}'$ be classes of structures over the relational signatures τ and τ', respectively. Let Φ be a strong first-order reduction from $\mathcal{C}$ to $\mathcal{C}'$, and let $L \subseteq \mathcal{C}$. Then*

$$L \in \underline{\mathcal{F}}(\mathcal{C}) \iff \textit{there is } L' \in \underline{\mathcal{F}}(\mathcal{C}') \textit{ with } \Phi(L) = L' \cap \Phi(\mathcal{C})$$

for all $\mathcal{F}$ among Σ_k, $\mathrm{B}(\Sigma_k)$, $\Sigma_k^{\mathrm{TC}(1)}$, $\mathrm{PFO}(\Sigma_k)$, $\mathrm{closed}(\Sigma_k)$.

If, additionally, $\Phi(\mathcal{C})$ is $\mathcal{F}$-definable, then

$$L \in \underline{\mathcal{F}}(\mathcal{C}) \iff \Phi(L) \in \underline{\mathcal{F}}(\mathcal{C}')$$

for all of the above choices of $\mathcal{F}$ as well as for Δ_k.

The monadic first-order reductions of [Cos93] are defined in a more syntactic flavour. More important, the definition of "monadic first-order reductions" is that it lacks item 4 of Definition 32. As a consequence, under the weaker assumption that $\Phi(L)$ is monadic first-order reducible to L, one can only conclude the directions "$\Leftarrow$" of the above theorem. This is formulated in [Cos93] for the class Σ_1, i.e. the existential fragment of monadic second-order logic.

For the easy direction "$\Rightarrow$", a formula φ over τ has to be transformed into a formula φ' over τ' such that φ' says over structures in $\Phi(\mathcal{C})$ the same as φ does for structures in $\mathcal{C}$. For this aim, we shall replace the atomic subformulas of φ by formulas that exist by item 4 in Definition 32, and we shall relativize first-order quantifications to the first of the n disjoint copies of the universe. We could also relativize the second-order quantifications to the first copy, but this is not necessary because the relativization of first-order quantifications implies that the value of second-order variables only matters on the first copy.

Proof of first claim of Theorem 33, "only if"-Part. Let $\mathcal{F}$ be any of the classes Σ_k, $\mathrm{B}(\Sigma_k)$, $\Sigma_k^{\mathrm{TC}(1)}$, $\mathrm{PFO}(\Sigma_k)$, $\mathrm{closed}(\Sigma_k)$. We will describe how to translate $\mathcal{F}$-formulas over τ into $\mathcal{F}$-formulas over τ'.

Let $\psi_1(x) = \exists x_2 \ldots \exists x_n \psi(x, x_2, \ldots, x_n)$, where ψ is chosen according to Definition 32. For an element x of the universe of a structure $\Phi(M)$ in the image of Φ, the formula $\psi_1(x)$ asserts that $x \in \{1\} \times \mathrm{dom}M$.

We show by induction that every formula φ over τ (say with free variables $X_1, \ldots, X_t, x_1, \ldots, x_m$) has the following property:

There is an MSO-formula φ' over τ' with the same free variables and belonging to the same of the above-mentioned classes as φ such that for all structures M in $\mathcal{C}$ and all $U_1, \ldots, U_t \subseteq \mathrm{dom}M$, $u_1, \ldots, u_m \in \mathrm{dom}M$ we have

$$\begin{array}{ll} & M \models \varphi[U_1, \ldots, U_t, u_1, \ldots, u_m] \\ \Longleftrightarrow & \Phi(M) \models \varphi'[\{1\} \times U_1, \ldots, \{1\} \times U_t, (1, u_1), \ldots, (1, u_m)]. \end{array}$$

So let us consider some MSO-formula φ , and assume that every less complex formula has this property.

In case $\varphi = Xx$ for some second-order variable X and a first-order variable x, let $\varphi' = \varphi$.

In case $\varphi = (x{=}y)$ for two first-order variables x, y, let $\varphi' = \varphi$.

In case $\varphi = r(y_1, \ldots, y_l)$ for some l-ary relation symbol r in τ, there exists a formula φ' with the desired property because Φ is a strong first-order reduction (item 4 from Definition 32).

In case $\varphi = \sigma \wedge \rho$, choose σ' and ρ' by induction and $\varphi' := \sigma' \wedge \rho'$. Similarly for $\vee$ instead of $\wedge$ and in case $\varphi = \neg\sigma$.

In case $\varphi = \exists x \sigma$, choose σ' by induction and let $\varphi' := \exists x(\psi_1(x) \wedge \sigma')$, i.e., first-order quantification is relativized to ψ_1.

In case $\varphi = \exists X \sigma$: Let $\varphi' := \exists X \sigma'$, where σ' is chosen by induction.

In case $\varphi = \mathrm{TC}(y, z, \sigma)$: Let $\varphi' := \mathrm{TC}(y, z, \psi_1(y) \wedge \sigma')$, where σ' is chosen by induction.

In any of the above cases φ' shows the desired property. □

The converse direction of the proof of Theorem 33 is more complicated. Item 3 of Definition 32 provides formulas that replace atomic subformulas of some φ' over τ'. But since in the universe of a Φ-image of a structure M there are n times as many elements as in M and quantifications may range over (subsets of) this larger universe, a formula over M will use n-times as many second-order variables and the same first-order variables together with built-in case distinctions concerning their membership in the different copies of $\mathrm{dom}M$.

We prepare the proof of direction "$\Leftarrow$" of Theorem 33 with some definitions and lemmas.

Definition 34 *Let $n \geqslant 1$. Let M and M' be, respectively, a τ- and a τ'-structure with* $\mathrm{dom}M' = [n] \times \mathrm{dom}M$.

Let $\varphi(X_1,\dots,X_t,x_1,\dots,x_m)$ be an $\mathrm{FO}^{\mathrm{TC}(1)}$-formula over τ' and $\varphi_\kappa(\overline{X_1},\dots,\overline{X_t},x_1,\dots,x_m)$ an $\mathrm{FO}^{\mathrm{TC}(1)}$-formula over τ for every $\kappa:[m]\to[n]$. (Here, the $\overline{X_i}$ are variable tuples of length n.)

Then the family $(\varphi_\kappa)_\kappa$ realizes *φ wrt. M and M' iff for all n-tuples $\overline{U_1},\dots,\overline{U_t}$ of subsets of $\mathrm{dom}M$, for all $u_1,\dots,u_m\in\mathrm{dom}M$, and all κ,*

$$\begin{aligned}&M\models\varphi_\kappa[\overline{U_1},\dots,\overline{U_t},u_1,\dots,u_m]\iff\\&M'\models\varphi[\textstyle\bigcup_{i\leqslant n}(\{i\}\times U_{1i}),\dots,\bigcup_{i\leqslant n}(\{i\}\times U_{ti}),(\kappa(1),u_1),\dots,(\kappa(m),u_m)].\end{aligned}$$

Let Φ be a strong first-order reduction from the class $\mathcal{C}$ of τ-structures into the class $\mathcal{C}'$ of τ'-structures. Let $\mathcal{F}$ be a class of formulas over τ. A formula $\varphi(X_1,\dots,X_t,x_1,\dots,x_m)$ over τ' is $\mathcal{F}$-realizable *with respect to Φ iff there is a family $(\varphi_\kappa(\overline{X_1},\dots,\overline{X_t},x_1,\dots,x_m))_\kappa$ of formulas in $\mathcal{F}$ that realizes φ wrt. M and $\Phi(M)$ for every structure M of $\mathcal{C}$.*

Lemma 35 *Let $n\geqslant 1$ and Φ be a strong first-order reduction of rank n. Let $\mathcal{F}$ be a class of τ-formulas. Let $\varphi(X_1,\dots,X_t,x_1,\dots,x_m)$ and $\psi(X_1,\dots,X_t,x_1,\dots,x_m)$ be formulas over τ' that are $\mathcal{F}$-realizable wrt. Φ.*

Then the following formulas are $\mathcal{F}$-realizable wrt. Φ, too:

1. *$\neg\varphi$, $\varphi\vee\psi$, provided $\mathcal{F}$ is closed under negation and disjunction, respectively;*
2. *$\exists x_m\varphi$, provided $\mathcal{F}$ is closed under disjunction and first-order quantification;*
3. *$\mathrm{TC}(x_p,x_q,\varphi)$ (where $p,q\leqslant m$ are distinct), provided $\mathcal{F}$ is closed under Boolean operations, first-order quantification, and application of the unary* TC*-operator;*
4. *$\exists X_t\varphi$, provided $\mathcal{F}$ is closed under existential monadic second-order quantification.*

Proof Let $(\varphi_\kappa)_{\kappa:[m]\to[n]}$ and $(\psi_\kappa)_{\kappa:[m]\to[n]}$ be families of $\mathcal{F}$-formulas (with free variables among $X_{11},\dots,X_{tn},x_1,\dots,x_m$) that realize φ and ψ, respectively, wrt. Φ.

ad 1 Obviously $(\neg\varphi_\kappa)_\kappa$ realizes $\neg\varphi$, and $(\varphi_\kappa\vee\psi_\kappa)_\kappa$ realizes $\varphi\vee\psi$.

ad 2 For $\kappa:[m-1]\to[n]$ and $i\leqslant n$ we define $\kappa(m\mapsto i)$ to be the extension of κ that maps m to i.

Then $\big(\exists x_m(\bigvee_{i\leqslant n}\varphi_{(\kappa(m\mapsto i))})\big)_{\kappa:[m-1]\to[n]}$ realizes $\exists x_m\varphi$ wrt. Φ.

ad 3 W.l.o.g. let $p = 1$ and $q = 2$. Let $\kappa : [m] \to [n]$. Depending on κ, we define τ-formulas σ_{ij}^{l} for $1 \leqslant i, j \leqslant n$ and $0 \leqslant l \leqslant n$ inductively over l as follows (reminding of the standard construction for regular expressions from non-deterministic finite automata):

$$\begin{aligned}
\sigma_{ij}^{0}(\overline{X}, \overline{x}) &= \begin{cases} \varphi_{\kappa(1\mapsto i)(2\mapsto j)}(\overline{X}, \overline{x}) & \text{if } i \neq j, \\ \varphi_{\kappa(1\mapsto i)(2\mapsto j)}(\overline{X}, \overline{x}) \vee (x_1 = x_2) & \text{else,} \end{cases} \\
\sigma_{ij}^{l}(\overline{X}, \overline{x}) &= \sigma_{ij}^{l-1} \vee \ \exists z, z' (\ \ \sigma_{il}^{l-1}(\overline{X}, x_1, z, x_3, \ldots, x_m) \\
&\qquad\qquad\qquad \wedge \mathrm{TC}(x_1, x_2, \sigma_{ll}^{l-1})(\overline{X}, z, z', x_3, \ldots, x_m) \\
&\qquad\qquad\qquad \wedge \sigma_{lj}^{l-1}(\overline{X}, z', x_2, x_3, \ldots, x_m))
\end{aligned}$$

Let $M \in \mathcal{C}$ and let $\overline{U_1}, \ldots, \overline{U_t}$ be n-tuples of subsets of dom$M$ and let us write U_j instead of $\bigcup_{i\leqslant n}(\{i\} \times U_{ji})$ for every $j \leqslant t$. Then one shows, inductively over l, the following property for every l, i, j:

$M \models \sigma_{ij}^{l}[\overline{U_1}, \ldots, \overline{U_t}, u_1, \ldots, u_m]$ iff there is a sequence α in $[n] \times \mathrm{dom}M$ that starts in (i, u_1), ends in (j, u_2), all intermediate components are in $[l] \times \mathrm{dom}M$, and if $(\nu, u), (\nu', u')$ are successive components of α, then $\Phi(M) \models \varphi[U_1, \ldots, U_t, (\nu, u), (\nu', u'), (\kappa(3), u_3), \ldots, (\kappa(m), u_m)]$.

Let $\varrho_\kappa = \sigma_{\kappa(1),\kappa(2)}^{n}$. Then $M \models \varrho_\kappa[\overline{U_1}, \ldots, \overline{U_t}, u_1, \ldots, u_m]$ iff $\Phi(M) \models \mathrm{TC}(x_1, x_2, \varphi)[U_1, \ldots, U_t, (\kappa(1), u_1), \ldots, (\kappa(m), u_m)]$.

Thus $(\varrho_\kappa)_\kappa$ realizes indeed $\mathrm{TC}(x_1, x_2, \varphi)$ wrt. Φ.

ad 4 We claim that $\left(\exists X_{t1} \ldots \exists X_{tn}(\varphi_\kappa)\right)_\kappa$ realizes $\exists X_t\varphi$ wrt. Φ.

Let $\overline{U_1}, \ldots, \overline{U_{t-1}}$ be n-tuples of subsets of dom$M$ and $u_1, \ldots, u_m \in \mathrm{dom}M$ and $\kappa : [m] \to [n]$.

$M \models (\exists X_{t1} \ldots \exists X_{tn}(\varphi_\kappa))[\overline{U_1}, \ldots \overline{U_{t-1}}, u_1, \ldots, u_m]$ iff there exist $U_{t1}, \ldots, U_{tn} \subseteq \mathrm{dom}M$ such that $M \models \varphi_\kappa[\overline{U_1}, \ldots, \overline{U_t}, u_1, \ldots, u_m]$ iff (by induction hypothesis) there exist $U_{t1}, \ldots, U_{tn} \subseteq \mathrm{dom}M$ such that $\Phi(M) \models \varphi[\bigcup_{i\leqslant n}(\{i\} \times U_{1i}), \ldots, \bigcup_{i\leqslant n}(\{i\} \times U_{ti}), (\kappa(1), u_1), \ldots, (\kappa(m), u_m)]$ iff (since every set $U \subseteq \mathrm{dom}\Phi(M)$ can be written as $\bigcup_{i\leqslant n}(\{i\} \times U_i)$ for some subsets U_i of dom$M$) $\Phi(M) \models (\exists X_t\varphi)[\bigcup_{i\leqslant n}(\{i\} \times U_{1i}), \ldots, \bigcup_{i\leqslant n}(\{i\} \times U_{t-1,i}), (\kappa(1), u_1), \ldots, (\kappa(m), u_m)]$. □

Lemma 36 *Let $\mathcal{F}$ be any of the classes Σ_k, $\mathrm{B}(\Sigma_k)$, $\Sigma_k^{\mathrm{TC}(1)}$, $\mathrm{PFO}(\Sigma_k)$, $\mathrm{closed}(\Sigma_k)$.*

Let Φ be a strong first-order reduction from the class $\mathcal{C}$ of τ-structures into the class $\mathcal{C}'$ of τ'-structures.

Every $\mathcal{F}$-formula $\varphi(X_1, \ldots, X_t, x_1, \ldots, x_m)$ over τ' is $\mathcal{F}$-realizable wrt. Φ.

Proof Let n be the rank of Φ. We argue by induction on the complexity of φ. Let us consider the atomic formulas first.

$X_i x_j$ is realized by $(X_{i,\kappa(j)} x_j)_\kappa$ because for every M, all n-tuples $\overline{U_1}, \ldots, \overline{U_t}$ of subsets of dom$M$, every $u_1, \ldots, u_m \in$ dom$M$, and every $\kappa : [m] \to [n]$ one has $\Phi(M) \models (X_i x_j)[\bigcup_{l \leqslant n}(\{l\} \times U_{1l}), \ldots, \bigcup_{l \leqslant n}(\{l\} \times U_{tl}), (\kappa(1), u_1), \ldots, (\kappa(m), u_m)]$ iff $(\kappa(j), u_j) \in \bigcup_l(\{l\} \times U_{il})$ iff $u_j \in U_{i,\kappa(j)}$ iff $M \models (X_{i,\kappa(j)} x_j)[\overline{U_1}, \ldots, \overline{U_t}, u_1, \ldots, u_m]$.

A family of formulas that realizes $r'(y_1, \ldots, y_l)$ for some l-ary relation symbol r' of τ' and variables $y_1, \ldots, y_l$ among $x_1, \ldots, x_m$ is provided by Definition 32, item 3.

A formula $x_i = x_j$ (where $i, j \leqslant m$) is realized by $(\varphi_\kappa)_\kappa$ with

$$\varphi_\kappa = \begin{cases} x_i = x_j & \text{if } \kappa(i) = \kappa(j) \\ \neg(x_i = x_i) & \text{else.} \end{cases}$$

Assuming as an induction hypothesis that all proper subformulas of a τ'-formula φ are realized by some adequate family of τ-formulas, we may use Lemma 35 to conclude that also φ is realized by some family of τ-formulas.

For example, if $\varphi(X_1, \ldots, X_t, x_1, \ldots, x_m)$ is a Σ_k-formula that is Σ_k-realizable wrt. Φ, then so is $\exists X_t \varphi$ by item 4 of Lemma 35.

Or if φ is $\mathrm{FO}^{\mathrm{TC}(1)}$-realizable, then so is $\mathrm{TC}(x_p, x_q, \varphi)$ by item 3 of Lemma 35.

This completes the proof of Lemma 36. □

Now we are ready to prove the converse direction of Theorem 33. We exploit Lemma 36 for sentences.

Proof of first claim of Theorem 33, "if"-Part. Let $\mathcal{F}$ be any of the classes Σ_k, $\mathrm{B}(\Sigma_k)$, $\Sigma_k^{\mathrm{TC}(1)}$, $\mathrm{PFO}(\Sigma_k)$, closed(Σ_k).

Let $L \subseteq \mathcal{C}$, $L' \in \underline{\mathcal{F}}(\mathcal{C}')$ with $L' \cap \Phi(\mathcal{C}) = \Phi(L)$. Choose a τ'-sentence φ in $\mathcal{F}$ such that $L' = Mod_{\mathcal{C}'}(\varphi)$.

By Lemma 36 (applied to the case of sentences, i.e. $t = m = 0$ and κ being the empty mapping) there is an $\mathcal{F}$-sentence $\varphi_\emptyset$ over τ such that

$$M \models \varphi_\emptyset \iff \Phi(M) \models \varphi$$

for every structure $M \in \mathcal{C}$. This implies $L = Mod_{\mathcal{C}}(\varphi_\emptyset) \in \underline{\mathcal{F}}(\mathcal{C})$.

This completes the proof of the first claim of Theorem 33. □

Proof of second claim of Theorem 33. The second claim for the syntactic formula classes Σ_k, $\mathrm{B}(\Sigma_k)$, $\Sigma_k^{\mathrm{TC}(1)}$, $\mathrm{PFO}(\Sigma_k)$, closed(Σ_k) is an immediate consequence of the first claim because these classes are closed under conjunction. By applying this equivalence with $\mathcal{F} = \Sigma_k$ twice, once to L and once to its complement, one obtains the second claim also for the case $\mathcal{F} = \Delta_k$. □

We can conclude the following:

Corollary 37 *Let $\mathcal{C}$, $\mathcal{C}'$ be classes of relational structures and Φ a strong first-order reduction from $\mathcal{C}$ to $\mathcal{C}'$. Then*

$$\underline{\mathcal{F}_1}(\mathcal{C}) \not\subseteq \underline{\mathcal{F}_2}(\mathcal{C}) \implies \underline{\mathcal{F}_1}(\mathcal{C}') \not\subseteq \underline{\mathcal{F}_2}(\mathcal{C}')$$

for all of the classes $\mathcal{F}_1$, $\mathcal{F}_2$ among Σ_k, $\mathrm{B}(\Sigma_k)$, $\Sigma_k^{\mathrm{TC}(1)}$, $\mathrm{PFO}(\Sigma_k)$, $\mathrm{closed}(\Sigma_k)$, for arbitrary $k \geqslant 0$.

If, additionally, $\Phi(\mathcal{C})$ is $\mathcal{F}_1$-definable, then the above implication holds also in case $\mathcal{F}_1$ equals Δ_k.

The proof is immediate because if L is a subset of $\mathcal{C}$ showing some non-inclusion over $\mathcal{C}$, then there is a set L' of $\mathcal{C}'$-structures with $L' \cap \Phi(\mathcal{C}) = \Phi(L)$ that shows the respective non-inclusion in the hierarchy over $\mathcal{C}'$.

In order to apply the above corollary to the classes of grids and (directed and undirected) graphs, we need the following proposition:

Proposition 38 *There are strong first-order reductions (1) from the class of grids to the class of finite directed graphs, (2) from the class of t-bit grids to the class of finite directed graphs (for every t), and (3) from the class of finite directed graphs to the class of finite undirected graphs.*

In all cases, the image of the reduction is Π_1-definable.

The first claim is, of course, a specialization of the second one. We will nevertheless show the three claims of the proposition separately. The approach is always the same: For the strong first-order reduction from $\mathcal{C}$ to $\mathcal{C}'$ we introduce a $\mathcal{C}'$-gadget that replaces each node of a $\mathcal{C}$-structure. The crucial point is that in the Φ-image of a structure there are no induced subgraphs isomorphic to the respective gadgets except for the gadgets themselves. That is why a first-order formula ψ (for item 2 of Definition 32) can be found that allows to fix these gadgets (simply by describing them).

In the following subsections we will show the three claims of Proposition 38.

From Grids to Graphs. For the first claim of Proposition 38, we define for every $R \in$ Grid the graph $\Phi(R) := (\{1,2\} \times \mathrm{dom}R, E)$ with

$$\begin{aligned} E = \quad & \{((1,x),(1,x)) \mid x \in \mathrm{dom}R\} \\ \cup \quad & \{((1,x),(2,x)) \mid x \in \mathrm{dom}R\} \\ \cup \quad & \{((2,x),(1,y)) \mid (x,y) \in S_1^R\} \\ \cup \quad & \{((2,x),(2,y)) \mid (x,y) \in S_2^R\} \end{aligned}$$

Figure 3 illustrates a "gadget" that replaces a grid node. The S_1- (respectively S_2-) edges of a grid are then coded by graph edges from 2- to 1-nodes (to 2-nodes, respectively).

$$
\begin{tikzcd}
(1,x) \arrow[loop above] \arrow[r] & (2,x)
\end{tikzcd}
$$

Figure 3: Gadget to Encode Grid-Node x in Directed Graphs

Now we give the formulas required to verify that Φ is indeed a strong first-order reduction. For item 2 of Definition 32 we use $\psi(x_1, x_2) = Ex_1x_1 \wedge Ex_1x_2 \wedge \neg Ex_2x_2$. Then the formulas for item 3 are:

$$
\begin{aligned}
\varphi^E_{(1,1)}(x_1, x_2) &= x_1{=}x_2, \\
\varphi^E_{(1,2)}(x_1, x_2) &= x_1{=}x_2, \\
\varphi^E_{(2,1)}(x_1, x_2) &= S_1x_1x_2, \\
\varphi^E_{(2,2)}(x_1, x_2) &= S_2x_1x_2.
\end{aligned}
$$

The formulas for item 4 of Definition 32 are:

$$
\begin{aligned}
\varphi^{S_1}(x_1, y_1) &= \exists x_2 \exists y_2 (\psi(x_1, x_2) \wedge \psi(y_1, y_2) \wedge Ex_2y_1), \\
\varphi^{S_2}(x_1, y_1) &= \exists x_2 \exists y_2 (\psi(x_1, x_2) \wedge \psi(y_1, y_2) \wedge Ex_2y_2).
\end{aligned}
$$

One easily verifies the properties required for a strong first-order reduction.

For the additional claim of Proposition 38 we need a Π_1-formula that defines the class $\Phi(\text{Grid})$ of graphs that are Φ-images of grids. A τ_{Grid}-structure R is called *irreflexive* if S_1^R and S_2^R are irreflexive. We start by showing that there is a Π_1-formula φ over signature τ_{Grid} that is true for an irreflexive τ_{Grid}-structure iff it is a grid.

φ asserts for a structure M over τ_{Grid} that, firstly, S_1 and S_2 are partial functions that commute; secondly that the "borders" look like in a grid, i.e. if $\{i, j\} = \{1, 2\}$ and whenever S_ixy, then x has a S_j-predecessor (-successor, respectively) iff y has; thirdly that there is exactly one vertex that has no successor (predecessor, respectively) at all; and fourthly that the structure is connected.

The first three assertions can be written as first-order formulas, whereas the last one as a Π_1-formula.

Now we note that the given first-order reduction Φ is in fact a strong first-order reduction from the class of irreflexive τ_{Grid}-structures into the class of graphs, and its image is Π_1- (even first-order) definable. Thus we may conclude from the additional statement of Theorem 33 that $\Phi(\text{Grid}) = \Phi(Mod_{\mathcal{C}}(\varphi))$ is Π_1-definable, which completes the proof of the additional claim of Proposition 38.

$$\begin{tikzcd}
(1,x) \arrow[loop above] \arrow[r, bend left] & (2,x) \arrow[l, bend left] \arrow[r] & (3,x) \arrow[r] & (4,x) \arrow[r] & (5,x)
\end{tikzcd}$$

Figure 4: Gadget to Encode 3-Bit Grid Node x in Directed Graphs

From Coloured Grids to Directed Graphs. For the strong first-order reduction from t-bit grids (for some $t \geqslant 0$) to directed graphs, i.e. for the second claim of Proposition 38, we need gadgets similar to the ones above but with the additional feature of coding some t-bit colour.

Let $M = \{(1,1),(2,1)\} \cup \{(i,i+1) \mid 1 \leqslant i \leqslant t+1\}$. For every t-bit grid R let $\Phi(R)$ be the graph with domain $[t+2] \times \mathrm{dom} R$ and edge set $\{((i,x),(j,x)) \mid (i,j) \in M\} \cup \{((i{+}2,x),(i{+}2,x)) \mid x \in X_i\} \cup \{((2,x),(1,y)) \mid (x,y) \in S_1^R\} \cup \{((2,x),(2,y)) \mid (x,y) \in S_2^R\}$.

So for some grid node x, the membership of x in X_i is coded by a loop edge on the $(i{+}2)$nd vertex of the corresponding gadget. Figure 4 illustrates the gadget for the case $k = 3$. Let $\psi(x_1, \dots, x_{t+2}) = \bigwedge_{(i,j)\in M} Ex_ix_j$. Then the formulas for item 3 of Definition 32 are:

$$\varphi^E_{(i,j)}(x_1,x_2) = \begin{cases} x_1{=}x_2 & \text{if } j = i+1 \vee i = j = 1, \\ S_1x_1x_2 \vee x_1{=}x_2 & \text{if } (i,j) = (2,1), \\ S_2x_1x_2 & \text{if } (i,j) = (2,2), \\ x_1{=}x_2 \wedge X_{i-2}x_1 & \text{if } i = j \geqslant 3, \\ \neg(x_1{=}x_1) & \text{else.} \end{cases}$$

The formulas for item 4 of Definition 32 are:

$$\begin{aligned} \varphi^{S_1}(x_1,y_1) &= \exists x_2 \dots x_{t+2}\, \exists y_2 \dots y_{t+2} \\ &\quad\ (\psi(x_1,\dots,x_{t+2}) \wedge \psi(y_1,\dots,y_{t+2}) \wedge Ex_2y_1) \\ \varphi^{S_2}(x_1,y_1) &= \exists x_2 \dots x_{t+2} \exists y_2 \dots y_{t+2} \\ &\quad\ (\psi(x_1,\dots,x_{t+2}) \wedge \psi(y_1,\dots,y_{t+2}) \wedge Ex_2y_2) \\ \varphi^{X_i}(x_1) &= \exists x_2 \dots x_{t+2}(\psi(x_1,\dots,x_{t+2}) \wedge Ex_{i+2}x_{i+2}) \end{aligned}$$

Using these formulas it is straightforward to verify that Φ is indeed a strong first-order reduction.

The additional claim that the image of this first-order reduction is Π_1-definable is shown in the same way as for the reduction from grids to graphs.

From Directed Graphs to Undirected Graphs. For the strong first-order reduction from directed graphs to undirected graphs, i.e. the third claim of Proposition 38, we define for every directed graph G the undirected graph $\Phi(G)$ with domain $[6] \times \mathrm{dom} G$ whose edges are as in Figure 5 plus an edge between $(1,x)$ and $(6,y)$ whenever (x,y) is an edge in G.

$$\begin{tikzcd}
 & (3,x) \arrow[r, dash] \arrow[d, dash] \arrow[dr, dash] & (4,x) \arrow[d, dash] & \\
(1,x) \arrow[r, dash] & (2,x) \arrow[r, dash] & (5,x) \arrow[r, dash] & (6,x)
\end{tikzcd}$$

Figure 5: Gadget to Encode Graph-Node x in Undirected Graphs

Formally: Let $M = \{\{1,2\},\{2,3\},\{3,4\},\{4,5\},\{5,2\},\{3,5\},\{5,6\}\}$ and $N = \{\{1,3\},\{1,4\},\{1,5\},\{2,4\},\{2,6\},\{3,6\},\{4,6\}\}$. The edge set of $\Phi(G)$ is given as $\{((i,x),(j,y)) \mid (x = y \wedge \{i,j\} \in M) \vee ((i,j) = (1,6) \wedge (x,y) \in E^G) \vee ((i,j) = (6,1) \wedge (y,x) \in E^G)\}$.

The formulas required to show that Φ is indeed a strong first-order reduction are the following: For item 2 of Definition 32 let

$$\begin{aligned}\psi(x_1,\dots,x_6) = \;& \forall z\,(Ezx_4 \to (x_3 = z \vee x_5 = z)) \\ & \wedge \textstyle\bigwedge_{\{i,j\}\in M}(Ex_ix_j) \wedge \bigwedge_{\{i,j\}\in N}(\neg Ex_ix_j).\end{aligned}$$

ψ fixes indeed the six nodes of a gadget (in the sense of item 2 of Definition 32). To verify this, let us consider an induced subgraph U of an undirected graph $\Phi((V,E))$ such that U satisfies ψ, say consisting of vertices $u_1,\dots,u_6$ as interpretations of $x_1,\dots,x_6$, respectively. If U constitutes a gadget of $\Phi((V,E))$, i.e., if $(u_1,\dots,u_6) = ((1,u),\dots,(6,u))$ for some $u \in V$, then we are done. Otherwise, the vertices u_2,u_3,u_4,u_5 have to be in $\{1,6\}\times V$, i.e., "endpoints" of at least two different gadgets. Thus in $\Phi((V,E))$, the node u_4 is adjacent with a vertex in $\{2,5\}\times V$ different from u_3 and u_5, contradicting the condition ψ.

The following formulas show item 3 of Definition 2:

$$\varphi^E_{(i,j)}(x,y) = \begin{cases} x = y & \text{if } \{i,j\} \in M, \\ Exy & \text{if } (i,j) = (1,6), \\ Eyx & \text{if } (j,i) = (1,6), \\ \neg(x = x) & \text{else.} \end{cases}$$

For item 4 of Definition 2 we need:

$$\begin{aligned}\varphi^E(x,y) = \;& \exists x_2 \dots x_6\, \exists y_1 \dots y_5 (\\ & \psi(x,x_2,\dots,x_6) \wedge \psi(y_1,\dots,y_5,y) \wedge Exy).\end{aligned}$$

These formulas show that Φ is a strong first-order reduction from the class of graphs to the class of undirected graphs.

For the additional claim of Proposition 38 we need a Π_1-formula that asserts for an undirected graph that it consists of disjoint copies of the gadget in Figure 5, possibly linked in the described way. This is done by the following (even first-order) formula:

$$\begin{aligned}
&\forall x \forall y \exists x_1 \dots x_6 \exists y_1 \dots y_6 \Big(\psi(x_1, \dots, x_6) \wedge \psi(y_1, \dots, y_6) \\
&\wedge \big(\textstyle\bigvee_{i \leqslant 6} x = x_i \big) \wedge \big(\textstyle\bigvee_{i \leqslant 6} y = y_i \big) \\
&\wedge \Big(Exy \rightarrow \big((x_1 = y_1) \vee (x = x_1 \wedge y = y_6) \vee (x = x_6 \wedge y = y_1) \big) \Big) \Big),
\end{aligned}$$

where ψ is as above.

5.2 Proof of Main Theorems

Now we are finally ready for the proofs of Theorems 1 and 3.

Proof of Theorem 1. The weak inclusion claim is clear by applying Remark 21.

By Theorem 4 and Theorem 5, the set $L_{f_{k+1}}$ for the function f_{k+1} of Theorem 5 is in $\underline{\Delta_{k+1}}(\text{Grid}) \setminus \underline{\mathrm{B}(\Sigma_k)}(\text{Grid})$ for every $k \geqslant 1$. This shows the claimed strictness for the class Grid. Corollary 37 and Proposition 38 yield this strictness for the classes Graph and UGraph.

For the second claim we first show that for every $k \geqslant 1$ there exist a $t \geqslant 1$ and a Σ_k-sentence φ over signature $\tau_{t\text{-Grid}}$ that is not equivalent to any Π_k-sentence.

Let $k \geqslant 1$. Since $\underline{\Sigma_{k+1}}(\text{Grid}) \not\subseteq \underline{\Sigma_k}(\text{Grid})$, there is a Σ_{k+1}-sentence φ over τ_{Grid} that is not equivalent (over grids) to any Σ_k-sentence. Let $\varphi = \exists X_1 \dots \exists X_t \neg\varphi'(X_1, \dots, X_t)$ for an appropriate Σ_k-formula $\varphi'(X_1, \dots, X_t)$ over τ_{Grid}. We consider φ' as a Σ_k-sentence over signature $\tau_{t\text{-Grid}}$. By choice of φ, the sentence φ' is not equivalent over the class of t-bit grids to any Π_k-sentence over $\tau_{t\text{-Grid}}$. This shows $\underline{\Sigma_k}(t\text{-Grid}) \not\subseteq \underline{\Pi_k}(t\text{-Grid})$.

Corollary 37 and Proposition 38 yield the respective non-inclusion for the classes Graph and UGraph. By duality, the converse non-inclusion also holds. □

Proof of Theorem 3. The first claim follows from Theorem 5, claims (3) and (4), together with Theorem 4.

For the second claim, let $k \geqslant 1$. By Theorem 5, claim (3) there exists a sentence over τ_{Grid} of the form $\exists \overline{X} \varphi(\overline{X})$, where φ is in $\mathrm{FO}^{\mathrm{TC}(1)}$ and $\overline{X}$ is a tuple, say of length t, such that $\mathit{Mod}_{\text{Grid}}(\exists \overline{X} \varphi(\overline{X})) \notin \underline{\Sigma_k}(\text{Grid})$. If we consider φ an $\mathrm{FO}^{\mathrm{TC}(1)}$-sentence over signature $\tau_{t\text{-Grid}}$, then clearly $\underline{\mathrm{FO}^{\mathrm{TC}(1)}}(t\text{-Grid})$ contains the set $\mathit{Mod}_{t\text{-Grid}}(\varphi(\overline{X}))$, which does not belong to $\underline{\Sigma_k}(t\text{-Grid})$. By Corollary 37 and Proposition 38 we obtain that $\underline{\mathrm{FO}^{\mathrm{TC}(1)}}(\text{Graph}) \not\subseteq \underline{\Sigma_k}(\text{Graph})$ and $\underline{\mathrm{FO}^{\mathrm{TC}(1)}}(\text{UGraph}) \not\subseteq \underline{\Sigma_k}(\text{UGraph})$.

Similarly, by Theorem 5, claim (4) we have that $\underline{\mathrm{PFO}(\Sigma_1)}(\text{Graph}) \not\subseteq \underline{\Sigma_k}(\text{Graph})$ and $\underline{\mathrm{PFO}(\Sigma_1)}(\text{UGraph}) \not\subseteq \underline{\Sigma_k}(\text{UGraph})$.

This completes the proof of Theorem 3. □

6 Conclusion

We have shown that the monadic quantifier alternation hierarchy over finite graphs is strict and that its structure resembles the classical hierarchies of recursion theory.

The hierarchy proof was based on finite grids as underlying models, automata theoretic ideas, and a transfer back to the domain of graphs. It turned out that over finite grids one reaches arbitrarily high levels of the monadic hierarchy already by means of Σ_1-definitions if in the kernel formulas either the unary transitive closure operator is admitted or if the transitive closures $\leqslant_1, \leqslant_2$ of the two successor functions over grids are included in the signature. (If even the binary transitive closure operator is admitted in the kernel formulas, a monadic second-order Σ_1-prefix suffices to define a set of grids which is not monadic second-order definable at all, cf. [MT97]).

Let us indicate some open questions.

We do not have a hierarchy proof for the monadic hierarchy over grids if the kernel formulas may involve the relations $\leqslant_1, \leqslant_2$ or even the unary transitive closure operator. However, as mentioned in Section 3, the present hierarchy proof can be saved if only the vertical order relation $\leqslant_1$ is adjoined to the signature of grids.

Also at higher levels of the monadic hierarchy one may proceed to more expressive classes of formulas. Recall the "closed hierarchy" of [AFS98], where one considers prefixes of monadic second-order and first-order quantifiers and classifies according to the alternation depth of the monadic second-order quantifiers. It is open whether a strict (or just infinite) hierarchy of graph properties is obtained when this alternation depth increases.

Finally, one might ask whether a natural notion of reducibility between monadic second-order (graph) properties exists which would allow the definition of complete problems for the levels of the monadic (or closed) hierarchy.

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