Synthesizability

A mathematical subject with an interpretation into the organic chemical synthesis

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Foreword

Which are the criteria to establish that a mathematical subject, which consists of mathematical objects and questions (or problems) about the objects, is interesting or important? In my opinion there are two criteria for this purpose. One criterion is that a sufficient number of mathematical authorities in the subject's field agree that the subject is interesting or important. This was, to mention a notable example, the case for the question whether the set theoretic continuum hypothesis follows or not from ZFC (Zermelo-Fraenkel axioms + axiom of choice).

The second criterion, that is hardly satisfied by the question in the example just given and is less compatible with the modern mathematical spirit than the first one, is fulfilled when the questions, which are part of the subject, are not in some way a mathematical triviality and their answer leads to the answer of questions about a major field outside of mathematics that a sufficient number of authorities in that field agree to declare interesting or important. In the past, until a few hundred years ago, almost exclusively this second criterion was used to consider a mathematical subject interesting or important. A good, albeit very particular, example for the application of this second criterion is the interest that existed for a solution to the problem of the bridges of Königsberg, which led to a mathematical problem, the problem which graphs are Eulerian, whose solution made it concretely impossible to travel a round trip traversing each of the bridges exactly once. Another example is the entire subject of real analysis, whose importance at the beginning, was given by the application to mechanics.

This second criterion is less compatible with the modern mathematical spirit, because it requires to fill in the gap between mathematics and the outside world, which has become much wider in the past century or so. It is often not clear at all when results in a mathematical subject can be used to answer questions about a field outside of mathematics.

So, for example, while the works of Gödel and of Turing on Turing Machines are considered to have been and, perhaps, to still be useful in the development of computer science, it is not obvious in which way precisely this usefulness happened. After all, no physical computer perfectly matches a Turing Machine or relies on the completeness of first-order logic to run.

The theory of Banach spaces has important applications to quantum mechanics, but nobody would realistically claim that the theory of Banach spaces represents the whole quantum mechanics in such a faithful way that it would be reasonable to identify the latter with the former. Therefore, if a mathematician, whose field is functional analysis, would develop a research subject within the theory of Banach spaces, it could be difficult to establish how useful results about this subject are in answering quantum mechanical questions.

But all these difficulties in determining whether results about a mathematical subject can be used to answer questions about a field outside of mathematics disappear when this field is represented by the objects of the mathematical subject with the thesis that these objects, due to the way in which they represent the field, are actually the field being represented, i. e. are identifiable with it. In this case, once the thesis is accepted, by the second criterion, if a sufficient number of authorities in the field outside of mathematics agree that certain questions about it are interesting or important and the representations of these questions are part of the subject, then the mathematical subject, provided its questions are not trivial, is interesting or important, too.

To go back to a previous example, the bridges of any town, whence also of Königsberg, can be easily represented by a graph (a mathematical object from graph theory) in such a way that it would be fully reasonable to claim that, from the view point of traveling across them, the graph is the bridges of the town. Stating that the graph is Eulerian is the same as stating that it is possible to travel a round trip crossing each bridge of the town exactly once. If the king of Prussia, to which Königsberg belonged, indisputably alone a sufficient authority in any field, would have been interested in knowing whether it was possible to travel a round trip crossing each bridge of Königsberg exactly once, then a complete characterization of Eulerian graphs, in a time in which graphs had essentially not been studied yet, would have been an interesting mathematical subject.

The second criterion to establish that a mathematical subject is interesting or important constitutes the core of the motivation for this book. The next two paragraphs explain why.

The question whether there is a chemical synthesis of a substance from other substances is probably the most important question in the field of chemical synthesis or even in chemistry, altogether. Historically chemistry is rooted in the desperate attempt of the alchemists, in the middle age, to obtain gold from other metals.

This books presents and examines, at an introductory level, with a strong focus on its logical and model theoretical aspects, a non-trivial, mathematical subject, at whose core lies a representation of the organic synthesis, as a field outside of mathematics, with the thesis that this representation, due to the, in this book, precisely described way in which it represents the organic synthesis, can be identified with the organic synthesis. With this thesis the question whether there is a chemical synthesis of an organic substance from other organic substances becomes a mathematical question. This question is also part of the core of this book's subject.

It becomes a mathematical question like, for instance, the question of the alchemists, whether it is possible to obtain gold from other metals, by a transformation achievable by them (i. e. a chemical transformation). A representation of a metal by an atom carrying exactly one symbol, with the thesis that atoms representing different metals carry different symbols, together with a representation, that it would be to tedious to describe in this foreword, of the transformations achievable by the alchemists, requiring the thesis that in a transformation neither the atoms nor their symbol change, would turn the question of the alchemists into a trivial, logical question, with a negative answer.

There are two possibilities to describe in which way mathematical objects represent a field outside of mathematics. The first possibility is to concretely assign a meaning in the field outside of mathematics to the mathematical objects and formulate the thesis about the field, first of all, for the assignment to exist, and, second, for the mathematical statements about the subject to be true with the assigned meaning.

The second possibility, which is the one adopted in this book, is to build the mathematical objects using the terminology of the field outside of mathematics, which determines their meaning in this field. The second possibility is not necessarily easier or more suitable than the first one, since it requires often to build mathematical objects with an awkward and overabundant terminology. Additionally, the non-mathematical meaning of the terminology might interfere with the logical reasoning. The advantage of the second possibility is that it allows to never leave mathematics.

The first possibility is, for example, the case, when the cartesian product $[0, n] \times \{n\} (n \in \mathbb{N}, n \neq 0)$ of the rational interval $[0, n]$ (whose usual order is $\leq$) and the set $\{n\}$, with the order $(r, n) \leq (s, n)$ if and only if $r \leq s$, represents a physical n meter beam, every physical n meter beam is represented by $[0, n] \times \{n\}$ with $\leq$, every $p \in [0, n] \times \{n\}$ represents a physical point of the n meter beam and the order $\leq$ represents the physical relation to be to the left. Then, among others, the theses must be adopted that n uniquely determines an n meter beam and that between any two distinct points of an n meter beam there is a third one, distinct from the two (said more exactly, for any distinct points a, b of an n meter beam, such that a is to the left of b, there is a point different from a and from b, that is to the left of b, to which a is to the left).

The second possibility is just to call the set $[0, n] \times \{n\}$ $(n \in \mathbb{N}, n \neq 0)$ with the previously defined order $\leq$ the n *meter beam*, every $p \in [0, n] \times \{n\}$ a *point* of it and define a point p of the n meter beam *to the left* of a point q of it if and only if $p \leq q$. In the case of this second possibility, no theses need to be adopted.

Summarized to an extreme, the objects of this book are the classes of structures that are derived by iterating an interpretation (fixed for the class), defined with parameters, starting from structures built by disjointly summing copies of structures from a set (fixed for the class) of finite structures. It is not known to me that those properties of the classes of structures derived in this way, that are examined in this book (i. e. whether they realize a sentence or are axiomatizable) have been examined in other works.

This book aims, to a significant extent, at suggesting in which directions its subject's core, which is, as previously written, a mathematical representation of the organic synthesis with the question, under which conditions there is a synthesis of a given compound from given compounds, can be developed and which issues from different mathematical disciplines (particularly from logic and model theory) arise from it. The results contained in the book form a solid base for a further and promising development.

We have chosen a policy that prevents as much as possible the repeated setting of variable values (for example with "let" or "assume" statements). This causes sometimes the scope of a variable setting to be a few pages long or even to last for the whole section.

Mathematical statements are lemmas, propositions or theorems. The end of their proofs is marked with $\diamondsuit$. We do not always refer explicitly, in a proof of a statement, to the previous basic results of this book (for example to Theorem 7.4 or to Proposition 7.1). Theorems are considered to have a higher relevance than propositions. Propositions could sometimes just be what in other works are remarks. A lemma in this work either becomes essentially redundant once the mathematical statement, it is a lemma of, has been proven or it is directly incorporated into a proof of a mathematical statement, which means, in this book, that it has no life outside of this proof.

Contents

0 Introduction

0.1 Synthesizability problems

The *synthesizability problem* for a reaction step notion $\mathcal{R}$ and a finite set $\mathcal{A}$ of compounds is the question:

> Given a compound C, is there a synthesis of C from $\mathcal{A}$ according to $\mathcal{R}$?

A reaction step notion is conceived as a finite set of reaction step rules. A synthesis according to $\mathcal{R}$ of C from $\mathcal{A}$ has in its initial stage only compounds from $\mathcal{A}$, C in its final stage and proceeds by steps according to the rules in $\mathcal{R}$. Equivalently we could restate the question:

> Given a compound C, is there is a reaction according to $\mathcal{R}$ having a left side whose compounds belong all to $\mathcal{A}$ and a right side of which C is a compound?

The *synthesizability problem* for the notion $\mathcal{R}$ and the compound C is the question:

> Given a finite set $\mathcal{A}$ of compounds, is there a synthesis of C from $\mathcal{A}$ according to $\mathcal{R}$?

Finally the *synthesizability problem* for a set $\mathcal{D}$ of notions is the question:

> Given $\mathcal{R} \in \mathcal{D}$ and compounds $A_1, \ldots, A_n, C$, is there a synthesis of C from $\{A_1, \ldots, A_n\}$ according to $\mathcal{R}$?

From the view point of computation theory, a *problem*, for some alphabet Σ and a set A of words over Σ, is the question, given a word w over Σ, whether w is in A or not. A problem is *solvable* iff (if and only if) there is a procedure the computes the right answer for every word over the problem's alphabet. In a graph theoretical problem the words over its alphabet code graphs. This book presents a list of graph theoretical problems and shows their solvability or unsolvability, whichever is the case.

Organic chemical terms, like (organic) formula, compound, sum of formulas, atom, charge, electron of a formula, being joined by a bond in a formula, carrying a charge in a formula, reaction step rule, synthesis, reaction, are strictly mathematically defined in this work and have, in their mathematical nature, nothing to do with organic chemistry. Nevertheless they are intended to have their ordinary chemical meaning. Whether they have it or not, is not a mathematical question, but a matter of opinion. Indeed, the likelihood that they do motivates the investigation presented in this book. This introduction attempts, without ever leaving mathematics, to let the chemical meaning emerge to an extent that can be evaluated from a chemical perspective. The price to pay for this attempt is that the order of the definitions, the terminology used in them as well as their number lack of high mathematical elegance.

0.2 Synthesis and reactions

The organic chemical terms are defined with parameters. These parameters, which depend on three distinct symbols $+$, $-$, $\bullet$, are

$m \in \mathbb{N}$,

a surjective function, called *multiplicity*, from a set, whose elements are called *bonds*, to $\{1, \ldots, m\}$,

a subset of $\{+, -, \bullet\}$, whose elements are called *implicit symbols*,

finitely many symbols, called *atomic*, different from the implicit symbols, that together with the implicit symbols form the *building symbols*, whose number is $n + 1$ ($n \in \mathbb{N}, n \geq m$),

a function, called *valence*, that assigns a $k \in \mathbb{N}$ to every atomic symbol and 1 to every implicit symbol.

The organic chemical terms are defined in Chapter 12 from the graph theoretical concepts introduced in Chapter 2 through the parameters listed above, a bijection s from $\{0, \ldots, n\}$ to the set of building symbols and the function $d\colon \{0, \ldots, n\} \to \mathbb{N}$, for which $d(i)$ is the valence of $s(i)$ ($0 \leq i \leq n$). These definitions act as an interface between the graph theoretical terminology and the chemical terminology, allowing a precise understanding of the intended chemical meaning. In particular they clarify what it means (in the representation of this book, of course) that an atom carries a charge or an electron and what a reaction step notion is. Most importantly, they are needed to proceed from the graph theoretical problems formulated in Chapter 3 to the synthesizability problems formulated at the beginning of this introduction.

Here are a few examples of definitions given in Chapter 12. A *sum of formulas* is defined as an m-bound n-multigraph with degree requirement d, a *formula* as a connected sum of formulas, a *compound* as an isomorphism class of formulas. Furthermore, and rather obviously, assuming $m \geq 2$, the atom a is *joined* to the atom b by a *double bond* (a bond of multiplicity 2) in the sum G of formulas simply iff $R_2^G(a, b)$. Perhaps less obviously, the atom a carries the positive charge b in G iff $R_1^G(a, b)$.

In this introduction we define the organic chemical terms directly, without falling back to the graph theoretical concepts of Chapter 2. This way of proceeding delivers to the reader two equivalent definitions of these terms.

We begin with the definition of a sum of arrangements. A sum of arrangements consists of finitely many, but at least one, *positions*, which are *atoms* or *implicit*. At every position exactly one building symbol *occurs*, which is atomic, if the position is an atom and implicit, if the position is implicit. A position at which $+$, $-$ respectively $\bullet$ occurs is called a *positive charge*, a *negative charge* respectively an *electron*. A *charge* is a positive or a negative charge. A sum of arrangements whose positions are all implicit, is called *implicit*. If it has an atom is called *atomic*.

The positions are pairwise *joined* (to each other) by exactly one bond or by no bond and *carry* a number (0 included) of positions. If two positions are joined by a bond, then they are different and both atoms. If a position carries a position, then, again, they are different and the second one is implicit. If an implicit position carries an implicit position, the the second one carries the first one. If $m = 0$ (i. e. there are no bonds), then no position carries a position. The *degree* of a position, which is the sum of the multiplicities of the bonds joining it to other atoms, increased by the number of positions, which it carries or by which it is carried, is less than or equal to the valence of the building symbol occurring at it.

Sum of arrangements G, H that do not have positions in common can be added in a quite natural way. This sum represents the sum appearing in any of the two sides of a (organic) chemical reaction. Their *sum* is the sum of arrangements whose set of positions is the union of the positions of G and H, that is equal to G on the positions of G, is equal to H on the positions of H and satisfies the condition that no atom of G is joined by a bond to an atom of H and no position of G carries or is carried by a position of H. Sum of arrangements G, H that transform into each other by adding to any of the two or to both an implicit sum of arrangements with new elements are called *atomically equivalent*.

A *semirule* is a pair of distinct sums of arrangements, of its *left* and *right side*, that satisfies the *fundamental reaction principles*, which state that, in passing from one side of the semirule to the other,

(1) no atoms are destroyed or created,

(2) they do not change neither the atomic symbol occurring at them nor their degree,

(3) no implicit position changes the implicit symbol occurring at it or the number of positions that carry it (0 or 1), if the position belongs to both sides.

Semirules, both sides of which are atomic, correspond to the intuitive idea of an organic chemical reaction step rule. Unfortunately, because the implicit positions in their two sides can differ, semirules are not quite suitable to be applied in the desired way. For this purpose we need the reaction step rules. A *reaction step rule*, or more simply a *rule*, is a pair of distinct sums of arrangements with the same positions, again of its *left* and *right side*, that also satisfies the fundamental reaction principles (1), (2), (3), in passing from one side of the rule to the other. We prefer the notation $G \to H$ for the rule (G, H) and call, in this introduction, a finite set of reaction step rules a *reaction step notion*.

From elementary graph theory it follows that for every semirule there is a rule whose left and right side are atomically equivalent respectively to the left and right side of the semirule, or, as we will write, that is *atomically equivalent* to the semirule. Hence every intuitive idea of an organic chemical reaction step rule is atomically equivalent to a rule.

If a sum of arrangements satisfies the requirement that the degree of every position of it is equal to the valence of the building symbol at that position, it is called a *sum of formulas*. A sum of arrangements is *connected* iff it is connected in the graph theoretical meaning, by considering that there is an edge between the positions a and b iff a bond joins a to b, a carries b or b carries a. An *isomorphism* from a sum of arrangements G to a sum of arrangements H is a bijection f from the set of positions of G to the set of positions of H that preserves the building symbol occurring at a position, the bond connecting a position to another one and the property that positions have to carry another one. More precisely f satisfies the conditions that for all positions a, b of G and all $1 \leq i \leq m$

(i) the same building symbol occurs in G at a as in H at $f(a)$,

(ii) a bond of multiplicity i joins a to b in G iff a bond of multiplicity i joins $f(a)$ to $f(b)$ in H,

(iii) a carries b in G iff $f(a)$ carries $f(b)$ in H.

A sum of arrangements G is *contained* in a sum of arrangements H iff every position of G is a position of H and H is equal to G on the positions of G. An isomorphism of G to a sum of arrangements contained in H is called an *embedding* of G into H.

A *formula* is a connected sum of formulas, a *compound* is an isomorphism class of formulas and an *equation* is a rule whose left and consequently also right side is a sum of formulas. Thus an equation satisfies the fundamental reaction principles. Instead of writing that a formula G belongs to a compound, we will also write that G is a *formula* of the compound or that the compound *has* the formula G. A *compound* of a sum of arrangements is a compound that has a formula contained in the sum of arrangements. If $F_0, \ldots, F_{k-1}$ are pairwise non-isomorphic formulas and $c_0, \ldots, c_{k-1} \in \mathbb{N}$ we denote by

$$c_0 F_0 + \ldots + c_{k-1} F_{k-1}$$

the class of all sums of pairwise disjoint isomorphic copies of $F_0, \ldots, F_{k-1}$, in which each F_i $(0 \leq i < k)$ has exactly c_i copies. It is clear that for every sum of formulas G there rule to the sum of arrangements G iff f is an embedding of K into G for which H is the shift, iterated k times, of G at $f(a_0), \ldots, f(a_{4k-1})$.

Since every equation is a reaction step rule and every reaction according to some notion is an equation, we also conclude that the shift has the capability to explain, step by step, every reaction according to some notion, or, written precisely, that for all reactions according to some notion there are $k \in \mathbb{N}$ and a sequence of $4k$ positions of the left side of the reaction such that the shift, iterated k times, of the left side of the reaction at those positions yields the right side of the reaction.

It is easy to establish, on the ground of the definition of the shift operation, given in Chapter 3, that there is a finite set of pairs $(K, (a_0, a_1, a_2, a_3))$, where $\{a_0, a_1, a_2, a_3\}$ is the set of positions of the sum of arrangements K, such that the sum of arrangements H is a shift of the sum of arrangements G with $H \neq G$ iff there is $(K, (a_0, a_1, a_2, a_3))$ in the set and an embedding f of K into G with $H = \mathrm{sh}(G, f(a_0), f(a_1), f(a_2), f(a_3))$. Therefore there is a reaction step notion, that we call *void*, such that the sum of arrangements H is a shift of the sum of arrangements G with $H \neq G$ iff H is the application of the notion to G.

Since, as we concluded before, the shift has the capability to explain, step by step, every reaction according to some notion, every reaction according to some notion is a reaction according to the void notion. This fact can be rephrased by stating that the shift is the most general reaction step notion.

We discovered previously that for every reaction step rule there is a sum of arrangements K, $k \in \mathbb{N}$ and positions $a_0, \ldots, a_{4k-1}$ of K with which the rule can be identified. We also explained why this discovery has a methodological relevance in the application of a reaction step notion. This discovery has a second advantage, that we have already used to define 1-fold rules: the classification of the reaction step rules on the ground of the model and, particularly, graph theoretical properties of their left side and the positions, with which the rule can be identified.

Several classes of reaction step rules have been defined in Chapter 12 in this way, for example the class of the additions, eliminations, substitutions, basic rules, unfragmented rules and k-fold rules.

This introduction began with the definition of three kinds of synthesizability problems. The synthesizability results, obtained in this book regarding them, can be summarized in the following way:

(I) If 3 building symbols have valence 1, 12 building symbols valence 2 and all bonds multiplicity 1 (i. e. $m = 1$), then for a finite set $\mathcal{R}$ of 2-fold additions, a 2-element compound C and a finite set $\mathcal{A}$ of at most 6-element compounds neither the synthesizability problem for $\mathcal{R}$ and $\mathcal{A}$, nor the synthesizability problem for $\mathcal{R}$ and C are solvable. This book gives a precise characterization of $\mathcal{R}$, C and $\mathcal{A}$.

(II) Four decidable sets of reaction step notions are presented for which the synthesizability problem is solvable. They are the class of the finite sets of 1-fold, unfragmented rules without eliminations, the class of the finite sets of rules that have a

1-fold factorization, all factors of which are not additions, the class of the (finite) sets of basic additions and the set with just the (non-empty, if $m \neq 0$) void notion.

(III) The question whether for the class of all finite sets of 1-fold rules or even 1-fold additions, the synthesizability problem is solvable or not remains open in this book.

The unsolvability results (I) are obtained by reducing two undecidable word problems for a semi-Thue system to them. The word problems themselves have been proven undecidable in a manner imitating Post's proof of the word problem's undecidability, i. e. by reducing the halting problem for a universal Turing machine to them. Both reduction are presented in Chapter 5.

Whether (I) answers or not the question about the decidability of the organic chemical synthesizability problem, is a matter of opinion and of perception of the physical world. If it should, then the undecidability result, although a little uncomfortable, has a much deeper philosophical meaning than the existence of a procedure: the meaning that higher goals in science, whence in life, can not be achieved by (following) effective rules, regardless how sophisticated these rules are.

[7] refers to an (unpublished) document in which the author claims that the organic chemical synthesizability problem is undecidable, as consequence of the undecidability of the word problem for semigroups. The work cited in [7] dedicates just a few lines to this result. It does not contain any explanation why the undecidability of the word

problem for semigroups implies the undecidability of the synthesizability problem. This explanation could be hardly given in the cited document, since there is no explanation in it of what a synthesis is. It actually looks like its idea is to reduce the synthesizability problem to the word problem, which does not prove the undecidability of the former.

For the first two classes in (II) the proof is easy and can be found in Chapter 3. The solvability for the third class, also shown in Chapter 3, to the contrary, should not be considered obvious. In fact, by dropping the condition that the additions are basic, the problem turns undecidable, as a consequence of (I).

The fourth case in (II) is interesting. The law of conservation of matter for a compound and a set of compounds states that every atomic symbol occurring at a position of a formula of the compound occurs at some position of a formula of a compound in the set. Assume that the highest valence of a building symbol is $\leq m$ and, in order to disregard the implicit symbols, that either only atomic symbols occur at any position of the formulas of the compound C or every implicit symbol occurs at some position of a formula of a compound in the set $\mathcal{A}$ of compounds. Then the criterion for the existence of a synthesis according to the void notion of C from $\mathcal{A}$ is simply the law of conservation of matter for C and $\mathcal{A}$. This claim is proven in Chapter 4. It emphasizes again the idea that the shift is the most general reaction step notion, since, for any reaction step notion, if there is a synthesis according to that notion of a compound from a set of compounds, then the law of conservation of matter holds for the compound and the set. Now, for the void notion, the converse holds, too: If the law of conservation of matter is valid for a compound and a set of compounds, then there is a synthesis according to the void notion of the compound from the set. This claim also implies at once that, for the void notion, a procedure deciding the synthesizability exists.

A few considerations may help putting (III) in the right perspective. A rule can be identified with its left side and, for some $k \in \mathbb{N}$, $4k$ positions of it. The application of the rule is then achieved by the execution, iteratively k times, of the shift at an image of the positions by means of an embedding of the left side. The shift itself is an operation at 4 positions. This book does not answer the natural question whether for the (decidable) set of all (up to isomorphism) reaction step notions, whose rules can be identified with their left side and exactly 4 positions, the synthesizability problem remains unsolvable. Should it, rather unexpectedly, turn out to be solvable, then so would be a very important particular case of the synthesizability problem. With the right philosophical approach to the organic chemical synthesis, one could say, if this particular problem would be decidable, that the whole organic chemical synthesizability is decidable.

0.3 Generalized reaction step notions

The graph theoretical problems have a natural generalization to model theoretical problems through the existence of a two-way correspondence between the reaction step notions, conceived as a finite set of rules, and the model theoretical interpretations, as they are defined in Chapter 7, narrowed down to the point of being m-bound reactional.

A notion yields the same application results as a corresponding interpretation and vice versa. This two-way correspondence is stated in Chapter 12 (Theorem 12.4) and proven from Theorem 10.3 in Chapter 10.

The approach to interpretations in this book is not completely standard. They are conceived as a way to transform a structure into another one and studied with the focus on the result obtained from iterating this transformation. When a structure interprets another one on the ground of a given interpretation, it can be considered the same as the other one, once the properties are intended in the meaning of the interpretation. To make a simple example, assuming that no red object is blue, a bag containing precisely 5 red and 3 blue objects can be considered the same as a bag with precisely 5 blue and 3 red objects, if we intend, only for the second bag, by "red" the meaning of "blue" and vice versa.

The correspondence between the reaction step notions and the interpretations means in particular that for any notion there exists an m-bound reactional interpretation that is equivalent to the notion, meaning that the right side of a reaction step according to the notion interprets its left side (by means of this interpretation) and whenever a sum of arrangements interprets a sum of arrangements, the former is an application of the notion to the latter. In the light of this interpretation, nothing changes from the right to the left side of a reaction step according to the notion.

The correspondence between notions and interpretations, being two-way, can be turned around: Not only every notion has an equivalent m-bound reactional interpretation corresponding to it, but every m-bound reactional interpretation has a corresponding equivalent notion. Hence the m-bound reactional interpretations could be another way to define the reaction step notions, conceived as a finite set of rules.

Additionally, we obtain that arbitrary interpretations that carry a sum of arrangements into a sum of arrangements, by satisfying the fundamental reaction principles, generalize the reaction step notions. We call them, in this introduction, *generalized reaction step notions*. *Synthesis*, *synthesis of* a compound *from* a set of compounds, (l-*step*) *reaction* and *reaction step* can be defined, in an obvious way, according to a generalized reaction step notion. The concept of synthesis can be generalized even more, by defining a *synthesis of* a first-order property of sums of arrangements *from* a set of compounds $\mathcal{A}$ according to a generalized reaction step notion φ as a synthesis $G_0, \ldots, G_l$ according to φ for which G_l has the property and all compounds of G_0 are in $\mathcal{A}$.

The *generalized synthesizability problem* for a generalized reaction step notion and a finite set $\mathcal{A}$ of compounds asks whether, given a first-order property of sums of arrangements, there is a synthesis according to the notion of the property from $\mathcal{A}$.

Through the model theoretical generalization of the graph theoretical problems, model theoretical and logical results become available to answer the original graph theoretical questions. The generalization opens the door to a wide area of logical and model theoretical topics. They all essentially turn around an investigation of the φ-*derivable* structures from a *combination* of $\mathcal{U}$, obtained by applying finitely many times (or a fixed finite number of times) the interpretation φ for a finite set L of relation symbols, using

$r \in \mathbb{N}$ additional constants, to a sum of pairwise disjoint isomorphic copies of structures belonging to the set $\mathcal{U}$ of structures over L.

A first investigation, based on logic, on this subject consists for example in determining the solvability (or unsolvability) of the following two problems for a finite set L of relation symbols, a quantifier-free interpretation φ for L and finite structures V_0, V_1 over L:

> Given a finite structure U over L, is there an extension of U that is φ-derivable from a combination of $\{V_0\}$? Is there an extension of V_1 that is φ-derivable from a combination of $\{U\}$?

In view of the result (I), as shown in Chapter 10 (Corollary 10.1), these problem are unsolvable for a certain finite set L of relation symbols, a certain quantifier-free interpretation φ for L a certain finite structure V_0 and a certain 2-element structure V_1, both over L.

The two problems are reduced in Chapter 11 to the finite satisfiability problem for certain sets of sentences. As a consequence we obtain that the finite satisfiability problem is not decidable for the classes $[\forall^{16} \wedge \exists^*, (14, 17)]_= \ \wedge \ \bigwedge_{0 \leq i < 13} \forall x \exists y S_i xy$ and $[\forall^* \wedge \exists^2, (14, 17)]_= \ \wedge \ \bigwedge_{0 \leq i < 13} \forall x \exists y S_i xy$, where S_i is a 2-placed relation symbol $(0 \leq i < 13)$.

A second investigation, based on model theory, on this subject is carried out in the Chapters 7 and 12. It deals with the φ-derivability in a fixed number of steps. It delivers a result that has a non-obvious consequence for the generalized synthesizability problem.

For every finite set L of relation symbols, interpretation φ for L, set $\mathcal{U}$ of structures over L and $l, i \in \mathbb{N}$, structures $U_0, \ldots, U_{k-1} \in \mathcal{U}$ and $c_0, \ldots, c_{k-1} \in \mathbb{N}$ are explicitly found in Section 7.2 (Theorem 7.7) (which, indeed, means effectively, if $\mathcal{U}$ is finite), with k less than some K depending only on φ, l and i, such that any l-equivalence type of a structure φ-derivable in $\leq i$ steps from a combination of $\mathcal{U}$ is already the type of a structure φ-derivable in $\leq i$ steps from a sum of pairwise disjoint isomorphic copies of $U_0, \ldots, U_{k-1}$ in which each U_i ($0 \leq i < k$) has at most c_i copies.

Three applications of this result are given in Section 7.3. These applications show that the values $U_0, \ldots, U_{k-1}$ and $c_0, \ldots, c_{k-1}$ explicitly found in Section 7.2 are surprisingly manageable and could be of practical interest. They require a good knowledge of the m-equivalence between structures. For this reason a whole chapter, Chapter 6, in which a new suitable condition for m-equivalence has been proven, has been dedicated to this subject.

The non-obvious consequence for the generalized synthesizability problem is that, for every generalized reaction step notion, set $\mathcal{A}$ of compounds, first-order property δ of sums of formulas and $i \in \mathbb{N}$, distinct compounds $A_0, \ldots, A_{k-1} \in \mathcal{A}$, having the formulas respectively $F_0, \ldots, F_{k-1}$, and $\bar{c}_0, \ldots, \bar{c}_{k-1} \in \mathbb{N}$ are explicitly found in Section 12.2 (Proposition 12.12) (effectively, if $\mathcal{A}$ is finite), depending only on the notion, $\mathcal{A}$, the quantifier rank of δ and i, with k less than some K depending only on the notion, the quantifier rank of δ and i, such that δ is synthesizable in $\leq i$ steps from $\mathcal{A}$ according to the notion iff there is a $\leq i$-step reaction $G \to H$ according to the notion for which H has the property δ and G is in the class $c_0F_0 + \ldots + c_{k-1}F_{k-1}$ with $c_i \leq \bar{c}_i$ $(0 \leq i < k)$.

The three applications, mentioned previously, have been themselves applied, in Section 12.2, to the synthesizability in a fixed number of steps according to a notion of a first-order property from a set of compounds. Again, the values $A_0, \ldots, A_{k-1}$ and $\bar{c}_0, \ldots, \bar{c}_{k-1}$ explicitly found in the applications of Section 12.2 are surprisingly manageable and, likely, of practical interest.

Finally, a third investigation, provided that $\mathcal{U}$ is a finite set of connected structures and φ invertible in a natural way, written correctly, weakly invertible, regards the axiomatizability (in this book always intended as first-order axiomatizability) of the class of all structures that are φ-derivable from a combination of $\mathcal{U}$. We show, in Chapter 9 (Corollary 9.8), that if the class is axiomatizable, then its theory (the set of all sentences in L holding in every structure of the class) is decidable.

Assuming that θ is a first-order sentence in L, instead of the combinations of $\mathcal{U}$, we consider the more general case of the models over L of θ and completely characterize in Corollary 9.4 the weakly invertible interpretations φ for L and the sentences θ in L for which the class of all structures that are φ-derivable from a model over L of θ is axiomatizable.

We also look at the case of the models over L of a theory T in L and, under the assumption that T and φ satisfy an additional condition, completely characterize in a very concise way in Theorem 9.8 the weakly invertible interpretations φ for L and the theories T in L for which the class of all structures that are φ-definable in (i. e. φ-derivable in 1 step from) a model over L of T is axiomatizable.

We do not want in this introduction to enter in the details about the additional condition that T and φ must satisfy for the proof of the characterization to be correct. It is anyways abundantly fulfilled, for example, by any theory and those "idempotent" interpretations that, applied twice in a row to a structure U, both times with the same values for the r additional constants, yield back the structure U.

A consequence, expressed in Proposition 12.15, of this third investigation, regarding the generalized synthesizability problem, is that, if φ is a weakly invertible generalized set of rules, $\mathcal{F}$ a finite set of formulas, $\mathcal{A}$ the set of all compounds having a formula in $\mathcal{F}$ and $\mathcal{C}$ the class of all sums of formulas G, for which there is a reaction $H \to G$ according to φ, where every compound of H is in $\mathcal{A}$, a sufficient condition for

> the generalized synthesizability problem for φ and $\mathcal{A}$ as well as the theory of $\mathcal{C}$ to be decidable,

is that the class of all structures φ-derivable from a combination of $\mathcal{F}$ (not just a finite combination) is axiomatizable or, equivalently, closed under ultraproducts.

If φ is quantifier-free and still weakly invertible and the class $\mathcal{C}$ of all structures that are φ-derivable from a model over L of the first-oder sentence θ in L is axiomatizable, Theorem 9.4 states that certain preservation properties of θ, that we explicitly indicate in the theorem, determine a corresponding, also explicitly indicated, preservation property of $\mathcal{C}$. In the case $r = 0$, which means that no additional constants are used in the application of φ, $\mathcal{C}$ is axiomatizable, whence the condition that it is axiomatizable can be dropped. Moreover Theorem 9.5 yields that in this case, if θ has one of the preservation properties indicated in Theorem 9.4 or a third property, explicitly indicated in Theorem 9.5, these properties are also true for $\mathcal{C}$.

Because these preservation properties play the role described above in the examination of the properties of the class $\mathcal{C}$ of structures φ-derivable from a structure in a class $\mathcal{D}$, in relation to the properties of $\mathcal{D}$, we dedicate to them the entire Chapter 8. More generally, the question how the (preservation) properties of $\mathcal{D}$ are reflected in the properties of $\mathcal{C}$ is faced a few times in this book.

0.4 Final considerations

Graphs have been, indeed, extensively used in chemistry for decades to represent organic formulas and organic molecules. The oldest book I know about graph theory in which this representation appears is [1]. The reader interested in the chemical approach to the application of graph theory to organic chemistry can consult, for example, [2], [3], [4], [5], [6], [7].

In these works graphs are used to investigate the molecular structure, in particular to determine the molecular properties from the properties of its graph representation. Other common uses of graph theory in chemistry include the creation of a smart nomenclature system or an adequate encoding of the molecule, suitable for being handled by a computer.

The reader should keep in mind that these works differ fundamentally from this book for at least two reasons. First reason: All chemical applications of the results in this book concern specifically and exclusively the organic chemical synthesis, that is the chemical transformation process that creates compounds from compounds. In particular, structural investigations of molecules, organic nomenclature or suitable molecular encodings are totally foreign to it. It has to be written that [7] suggests and discusses graph transformation as a way to represent organic reactions, but does not introduce a graph theoretical representation of the transformation that can be mathematically examined. Second and most important reason: This book is a book in mathematics. Arguments, concepts or facts from chemistry, that are not mathematical, do not play any role whatsoever in the achievement of any result contained in it.

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1 Preliminaries

Chapter 1 outlines the mathematical prerequisites needed to tackle the book. These prerequisites belong mostly to the fields of logic and model theory. A part of a few exceptions (for example, the U-extension of V or the combinations of $\mathcal{U}$) they are standard designations of these fields. More than half of the abbreviations that are used throughout the book are defined in this chapter.

As usual $\mathbb{N}$ is the set of the natural numbers $0, 1, 2, \ldots$. $\in$, $\subseteq$ are the set-theoretic element respectively subset relations. $\emptyset$, $A \cup B$, $A \cap B$, $A \setminus B$ denote respectively the empty set, the union of the sets A and B, their intersection and their difference (the complement of B in A). $\bigcup A$, $\bigcap A$ are the union of A (set of all elements of an element of A) respectively the intersection of A (set of all elements of every element of A). A^n is the set of all n-tuples of elements of the set A. The cardinality of A is written $|A|$. A *choice set* of a set A (of sets) is a set $X \subseteq \bigcup A$ with $|X \cap Y| = 1$ for all $Y \in A$. R is an *n-placed relation* over A $(n \in \mathbb{N})$ iff either $R(a_0, \ldots, a_{n-1})$ holds or it does not, for all $a_0, \ldots, a_{n-1} \in A$. $\operatorname{dom}(f)$ and $\operatorname{rg}(f)$ denote the domain and the range, respectively, of the function f. The identity function with domain A is denoted by id_A, the restriction of the function f to A, with $A \subseteq \operatorname{dom}(f)$, by $f|A$ and the composition of the functions f, g by $f \circ g$. $f\colon A \to B$ (f is a function from A to B) means that f is a function with $\operatorname{dom}(f) = A$ and $\operatorname{rg}(f) \subseteq B$. f is an *n-placed function* over A $(n \in \mathbb{N})$ iff f is a function with $A^n \subseteq \operatorname{dom}(f)$ and $\operatorname{rg}(f|A^n) \subseteq A$.

p is an *l-sequence* iff $p = p_0, \ldots, p_{l-1}$ ($l \in \mathbb{N}$). l is called the *length* of the l-sequence p. A *finite sequence* is an l-sequence for some $l \in \mathbb{N}$. A *sequence* is either finite or a function $p_0, p_1, p_2, \ldots$ with domain $\mathbb{N}$. Let p be an l-sequence and q an m-sequence. We denote the $(l+m)$-sequence $p_0, \ldots, p_{l-1}, q_0, \ldots, q_{m-1}$, when the context excludes ambiguities, by p, q. We call a sequence whose range is contained in the set A a *sequence* to A.

We assume a basic knowledge in logic and model theory as it can be acquired from several textbooks [1], [2], [3], [4], [5]. The logical conjunction (and), disjunction (or), negation (not), the universal quantifier (for all) and the existential quantifier (there is) are denoted respectively by $\wedge, \vee, \neg, \forall, \exists$. $\bigwedge, \bigvee$ denote the conjunction respectively disjunction of a set of formulas. A *symbol* is exactly one of the following three objects: a *relation symbol*, a *function symbol* or a *constant*. Every relation (or function) symbol F is n-placed for exactly one $n \in \mathbb{N} \setminus \{0\}$, denoted by ν_F. All sentences and formulas are intended to be first-order, unless there is a reason against it. As usual $\psi(x_0, \ldots, x_{k-1})$ means that all variables occurring free in the formula ψ are among $x_0, \ldots, x_{k-1}$. Square brackets, as in $\psi[y_0, \ldots, y_{i-1} : z_0, \ldots, z_{i-1}]$ are used to represent a variable substitution in a formula $\psi(x_0, \ldots, x_{k-1})$. If $y_0, \ldots, y_{i-1} = x_0, \ldots, x_{i-1}$, we may simply write $\psi[z_0, \ldots, z_{i-1}]$ for the substituted formula; if $y_0, \ldots, y_{i-1} = x_0, \ldots, x_{k-1}$, simply $\psi(z_0, \ldots, z_{k-1})$. Square brackets are also used to represent the substitution of subformulas, as in $\psi[Rt_0 \ldots t_{\nu_R} : \varphi]$. The *quantifier rank* of a formula ψ, $\mathrm{qr}(\psi)$, is recursively defined in the usual way starting from the atomic formulas. [4] [5]

Let L be a set of symbols. R^U is a ν_R-placed relation over the domain $\mathrm{dom}(U)$ of the structure U over L , $c^U \in \mathrm{dom}(U)$ and f^U is a ν_f-placed function over $\mathrm{dom}(U)$, for any relation symbol $R \in$ L, any constant $c \in$ L and any function symbol $f \in$ L. $\mathrm{dom}(U)$ is always assumed to be non-empty. If $\mathrm{L}_0 \subseteq \mathrm{L}$, the reduct of U to L_0 is denoted by $U \restriction \mathrm{L}_0$. If $A \subseteq \mathrm{dom}(U)$, (U, A) indicates the expansion of U with the elements of A. Every $a \in A$ is intended as a constant and interpreted by itself (i.e. $a^{(U,A)} = a$). If U is a structure over L and $S \notin$ L a symbol, we use the notation $(U, (S\colon F))$ for the structure V over $\mathrm{L} \cup \{S\}$ with $V \restriction \mathrm{L} = U$ and $S^V = F$. A structure U over L where every element of its domain is the interpretation in U of a term in L without variables is called *canonical*.

Let U, V be structures over the set L of relation symbols or constants. A *homomorphism* from V to U is a mapping $f\colon \mathrm{dom}(V) \to \mathrm{dom}(U)$ that satisfies for all constants c$\in$ L, all relation symbols $R \in$ L and all $v_0, \dots, v_{\nu_R - 1} \in \mathrm{dom}(V)$

$$c^U = f(c^V);$$

$$\text{if } R^V(v_0, \dots, v_{\nu_R-1}), \text{ then } R^U(f(v_0), \dots, f(v_{\nu_R-1})).$$

A homomorphism f from V to U that satisfies for all relation symbols $R \in$ L and all $v_0, \dots, v_{n-1} \in \mathrm{dom}(V)$

$$R^V(v_0, \dots, v_{\nu_R-1}), \text{ if } R^U(f(v_0), \dots, f(v_{\nu_R-1}))$$

is called *strict*. An *embedding* of (or from) V into U is a strict, injective homomorphism from V to U. An embedding from V into U that is surjective to $\mathrm{dom}(U)$ is called an *isomorphism* from V to U. V is said to be *embedded* into U respectively *isomorphic* to U, written $V \cong U$, if there is an embedding of V into U respectively an isomorphism from V to U. V is called a *substructure* of U (or *contained* in U) or U an *extension* of V (or *extending* V), written $V \subseteq U$ or $U \supseteq V$, iff the identity function $\mathrm{id}_{\mathrm{dom}(V)}$ is an embedding from V into U. If U is canonical and there is a homomorphism f from U to V, then f is unique and denoted by $e_{U,V}$.

Let L be a set of relation symbols and U, V structures over L.

If $\emptyset \neq A \subseteq \mathrm{dom}(U)$, the substructure of U whose domain is A is denoted by $U|A$. We define $U|\emptyset = \emptyset$. A *partial isomorphism* from V to U is either the empty function $\emptyset$ or an embedding from a substructure of V into U. For an injective f: $\mathrm{dom}(V) \to \mathrm{dom}(U)$, the U*-extension* of V by f is the structure W over L with $\mathrm{dom}(W) = \mathrm{dom}(U)$, into which f is an embedding from V, satisfying for all $R \in$ L and all $u_0, \ldots, u_{\nu_R-1} \in \mathrm{dom}(U)^{\nu_R} \backslash \mathrm{rg}(f)^{\nu_R}$

$$R^W(u_0, \ldots, u_{\nu_R-1}) \text{ iff } R^U(u_0, \ldots, u_{\nu_R-1}).$$

Let $\mathcal{U}$ be a non-empty set of structures over L with pairwise disjoint domains (i.e. $\mathrm{dom}(U) \cap \mathrm{dom}(V) = \emptyset$ for distinct $U, V \in \mathcal{U}$). The *sum* $\sum\mathcal{U}$ of $\mathcal{U}$ is defined to be the structure U over L with $\mathrm{dom}(U) = \bigcup\{\, \mathrm{dom}(V) \,|\, V \in \mathcal{G}\}$ satisfying for all $R \in$ L and all $u_0, \ldots, u_{\nu_R-1} \in \mathrm{dom}(U)$:

(i) For all $V \in \mathcal{U}$, if $u_0, \ldots, u_{\nu_{\mathbf{R}}-1} \in \mathrm{dom}(V)$,

$$R^U(u_0, \ldots, u_{\nu_R-1}) \text{ iff } R^V(u_0, \ldots, u_{\nu_R-1}).$$

(ii) If $\{u_0, \ldots, u_{\nu_R-1}\} \not\subseteq \mathrm{dom}(V)$ for all $V \in \mathcal{U}$,

$$\text{not } R^U(u_0, \ldots, u_{\nu_R-1}).$$

$\sum \mathcal{U}$ is written also $U \oplus V$, if $\mathcal{U} = \{U, V\}$ (thus $U \oplus U = U$). We define $\emptyset \oplus U = U \oplus \emptyset = U$.

For a structure U over L we call $A \subseteq \mathrm{dom}(U)$ *closed* in U iff $U = U|A \oplus U|(\mathrm{dom}(U) \setminus A)$. A *closed substructure* of U is a substructure of U whose domain is closed in U.

Let $\mathcal{U}$ be a class of structures over L. A *combination set* of $\mathcal{U}$ is a set $\mathcal{V} \neq \emptyset$ of structures over L with pairwise disjoint domains satisfying the condition that every $V \in \mathcal{V}$ is isomorphic to some $U \in \mathcal{U}$. A *combination* of $\mathcal{U}$ is a sum $\sum \mathcal{V}$ for some combination set $\mathcal{V}$ of $\mathcal{U}$. Said differently, a combination of $\mathcal{U}$ is the sum of a non-empty set of pairwise disjoint isomorphic copies of elements of $\mathcal{U}$. We denote the class of all combinations of $\mathcal{U}$ by $\mathrm{cmb}(\mathcal{U})$. A *combination* of a structure U over L is just a combination of $\{U\}$. If in the definition of a combination of $\mathcal{U}$ we add the requirement that $|\mathcal{V}| = m \in \mathbb{N}$, we call $\sum \mathcal{V}$ an *m-combination* of $\mathcal{U}$. A *finite-combination* of $\mathcal{U}$ is an m-combination of $\mathcal{U}$ for some $m \in \mathbb{N}$.

A *combination function* over $\mathcal{U}$ is a function α with $\mathcal{U} \subseteq \mathrm{dom}(\alpha)$, $\alpha(U)$ a cardinal number for all $U \in \mathcal{U}$ and $\alpha(U) = \alpha(V)$ for all $U \cong V$ in $\mathcal{U}$. Let α be a combination function over $\mathcal{U}$. A *combination set* of $\mathcal{U}$ *with coefficients* α is a combination set $\mathcal{V}$ of $\mathcal{U}$ such that $|\{V \in \mathcal{V} \mid V \cong U\}| = \alpha(U)$ for every $U \in \mathcal{U}$. A *combination* of $\mathcal{U}$ *with coefficients* α is a sum $\sum \mathcal{V}$ for a combination set $\mathcal{V}$ of $\mathcal{U}$ with coefficients α. Obviously any two combinations of $\mathcal{U}$ with coefficients α are isomorphic. If β is a combination function over $\mathcal{U}$, we call a combination of $\mathcal{U}$ with coefficients α a *combination* of $\mathcal{U}$ *with coefficients* $\leq \beta$ iff $\alpha(U) \leq \beta(U)$ for all $U \in \mathcal{U}$.

$\models$ denotes the semantical satisfaction relation between a class of structures and a formula. If $\mathcal{C}$ is a class of structures over the set L of symbols, the set of all sentences in L that hold in all structures in $\mathcal{C}$ is called the *theory* of $\mathcal{C}$ and denoted by $\mathrm{Th}(\mathcal{C})$. If $\mathcal{C}$ is empty, L is not uniquely determined. In this trivial case L will simply be the underlying set of symbols, in the realm of which we are situated. The class of all structures over L that satisfy a set T of (first-order) sentences in L, also called a *(first-order) theory* in L, is denoted by $\mathrm{mod}^{\mathrm{L}}(\mathrm{T})$. For a sentence ψ in L it will be safe for us to abbreviate $\mathrm{mod}^{\mathrm{L}}(\{\psi\})$ by $\mathrm{mod}^{\mathrm{L}}(\psi)$. A theory T in L *axiomatizes* a class $\mathcal{C}$ of structures over L iff $\mathcal{C} = \mathrm{mod}^{\mathrm{L}}(\mathrm{T})$. A sentence ψ in L *axiomatizes* $\mathcal{C}$ iff $\mathcal{C} = \mathrm{mod}^{\mathrm{L}}(\psi)$. If T' is a theory in L, we write that T or ψ *axiomatizes* T' instead of $\mathrm{mod}^{\mathrm{L}}(\mathrm{T}')$. $\mathcal{C}$ is *axiomatizable* iff there is a (first-order) theory in L that axiomatizes $\mathcal{C}$.

We might need the next definition, too. A theory in L *axiomatizes in the finite* a class $\mathcal{C}$ of structures over L iff $\mathcal{C}$ is the class of all finite models over L of the theory. We denote by $\mathcal{C}^{\mathrm{f}}$ the class of all finite structures in $\mathcal{C}$.

The structures U, V over the set L of symbols are *elementarily equivalent*, $U \equiv V$, iff they satisfy the same sentences in L, or, said differently, iff $\mathrm{Th}(U) = \mathrm{Th}(V)$ ($\mathrm{Th}(U)$ is short for $\mathrm{Th}(\{U\})$). U, V are *m-equivalent*, $U \equiv_m V$, iff they satisfy the same sentences in L of quantifier rank $m \in \mathbb{N}$. In Chapter 6 we will refine the following definition of k, m-equivalence ($k, m \in \mathbb{N}$). U, V are *k, m-equivalent*, $U \equiv_{k,m} V$, iff for all $u_0, \ldots, u_{k-1} \in \mathrm{dom}(U)$ there are $v_0, \ldots, v_{k-1} \in \mathrm{dom}(V)$ and vice versa such that $U, (c_i\colon u_i)_{0 \le i < k} \equiv_m V, (c_i\colon v_i)_{0 \le i < k}$ ($c_0, \ldots, c_{k-1}$ constants). We notice immediately that, if L is finite, because of Ehrenfeucht's Theorem, U, V are $1, m$-equivalent iff they are $m+1$-equivalent and that, if they are $m+k$-equivalent, then they are k, m-equivalent. The second conclusion can be also proven simply by using the m-Hintikka formulas in L [2] [5].

An embedding f from V into U is called *elementary* iff $(V, \mathrm{dom}(V)) \equiv (U, (v : f(v))_{v \in \mathrm{dom}(V)})$. V is an *elementary substructure* of U or U an *elementary extension* of V, written $V \preceq U$ or $U \succeq V$, iff $\mathrm{id}_{\mathrm{dom}(V)}$ is an elementary embedding from V into U. U is *i-sandwiched* by V $(i \ge 1)$ iff there are structures $U_0, \ldots, U_{i-1}$ over L with

$V \subseteq U_0 \subseteq \ldots \subseteq U_{i-1}$,

U is elementarily embedded into U_0,

$U_j \preceq U_{j+2}$ $(0 \le j < i-2)$ and

$V \preceq U_1$, if $i \ge 2$.

U is *i-filled* with V iff V is i-sandwiched by U. A class of structures over L is *preserved under i-sandwiches* iff for all structures U, V over L, if U is in the class and U is i-sandwiched by V, then V is in the class. It is *preserved under i-fillings* iff for all structures U, V over L, if U is in the class and U is i-filled with V, then V is in the class.

Let α be an ordinal and U_γ a structure over L for all ordinals $\gamma < \alpha$. We call $(U_\gamma)_{\gamma<\alpha}$ a *chain of structures* iff $U_\gamma \subseteq U_\delta$ for all ordinals $\gamma \le \delta < \alpha$. We assume the well known definition of the union $\bigcup (U_\gamma)_{\gamma<\alpha}$ of a chain $(U_\gamma)_{\gamma<\alpha}$ of structures (if needed, see for example [1]). A class $\mathcal{C}$ of structures over L is *preserved under chains* iff, for all chains $(U_\gamma)_{\gamma<\alpha}$ of structures with $U_\gamma \in \mathcal{C}$ for all ordinals $\gamma < \alpha$, the union of $(U_\gamma)_{\gamma<\alpha}$ is in $\mathcal{C}$.

The *(primitive) type* $\Delta_{U,u}$ of the k-sequence u to $\mathrm{dom}(U)$ in the structure U over the set L of relation symbols or constants is the conjunction of all atomic or negated atomic formulas $\xi(x_0, \ldots, x_{k-1})$ in L with $U \models \xi[u]$. A *(primitive) k-type* of U is the type of some k-sequence u to $\mathrm{dom}(U)$ in U. A *(primitive) k-type* of L is a k-type of some structure W over L. If U is finite, we denote by Δ_U, for a surjective k-sequence u to $\mathrm{dom}(U)$, the sentence $\exists y_0 \ldots \exists y_{k-1} \Delta_{U,u}$.

We assume a basic familiarity with recursion theory, computation and Turing machines [6], [7]. An alphabet is defined to be finite. Let Σ be an alphabet and w, v be in the set Σ^* of all words over Σ. $|w|_\Sigma$ is the length of w (with respect to Σ). w is a *subword* (with respect to Σ) of v iff $v = swt$ for some $s, t \in \Sigma^*$ (sw denotes the concatenation of s, w). A *problem* (in Σ) is for some $A \subseteq \Sigma^*$ the question, given a word over Σ, whether the word is in A or not. A problem is *solvable* iff there is a procedure (or, equivalently, a Turing machine) that computes the (correct) answer, yes or no. A class of finite structures over a finite set of symbols is *decidable* iff the set of all structures with domain $\{0, \ldots, n\}$ ($n \in \mathbb{N}$) that are isomorphic to a structure in the class is decidable.

We define the words π_i, σ_i ($i \in \mathbb{N}$) over the 2-letter alphabet $\{\forall^*, \exists^*\}$ in the following way:

π_0, σ_0 are the empty word. $\pi_{i+1} = \forall^* \sigma_i$, $\sigma_{i+1} = \exists^* \pi_i$ ($i \in \mathbb{N}$).

Let S be a set of symbols. We denote by Π_i^{S} respectively Σ_i^{S} the set of all prenex sentences in S with a prefix type π_i respectively σ_i, where $\forall^*$ respectively $\exists^*$ means any word over $\{\forall\}$ respectively $\{\exists\}$.

1.1 Equivalence relations

The equivalence relation $\equiv_{k,r,m}$, weaker than $\equiv_{r,m}$, will play an important role later in the Chapters 6 and 7. For its investigation we will use several definitions and propositions regarding equivalence relations in general. These definitions and propositions are the subject of this section.

As usual an *equivalence relation* over the set A is a 2-placed relation Q over A such that $A = \emptyset$ or the structure $(A, S{:}Q)$ (S 2-placed relation symbols) satisfies

$$\forall xyz(Sxx \wedge (Sxy \to Syx) \wedge ((Sxy \wedge Syz) \to Sxz)).$$

Let Q be an equivalence relation over the set A. A/Q denotes the set of all *equivalence classes* C_a (of a) ($a \in A$) *modulo* Q, where C_a is the set of all $b \in A$ with $Q(a,b)$. For $B \subseteq A$ and $i \in \mathbb{N}$ we denote by $< B >_{i,Q}^{A}$ the union of B and the set of all $a \in A$ that have Q with $> i$ elements in B. Q is *finer* (*over* A) than the equivalence relation R over A iff $Q(a,b)$ implies $R(a,b)$ for all $a, b \in A$. $B, C \subseteq A$ are called *Q-equivalent* iff the same Q types belong to them or, written more properly, iff for every $a \in B$ there is $b \in C$ with $Q(a,b)$ and vice versa.

Proposition 1.1 *$B, C \subseteq A$ are Q-equivalent iff for all choice sets D, E of B/Q respectively C/Q there is a bijection F from D to E with $Q(F(a), a)$ for all $a \in D$.*

Proof Obvious. $\diamondsuit$

This book will often deal with equivalence relations over classes, like $\cong$ or $\equiv$. The definitions referring to them can be easily acquired from the definitions given above, referring to an equivalence relation over a set, but the reader should be aware of the fact that the definitions above of an equivalence relation Q over A and of A/Q are not correct, if A is a class and not a set.

Let L be a set of relation symbols, $\mathcal{U}$ a set of structures over L and E be an equivalence relation over the class $\bar{\mathcal{U}}$ of all structures isomorphic to a structure in $\mathcal{U}$ with the property that $\cong$ is finer than E. If $\mathcal{V} \subseteq \bar{\mathcal{U}}$ is a set and $U \in \mathcal{U}$ we define

$$\alpha^{\mathcal{V}}_{E,\mathcal{U}}(U) = |\{V \in \mathcal{V} \mid E(V, U)\}|.$$

Clearly $\alpha^{\mathcal{V}}_{E,\mathcal{U}}$ is a combination function over $\mathcal{U}$.

The m-sequence Q of equivalence relations over A ($m \in \mathbb{N}$) is called *increasing* (*over* A) iff Q_i is finer (over A) than Q_j for all $0 \leq i \leq j < m$. If Q is an increasing m-sequence of equivalence relations over A and $0 \leq i \leq m$, we call the i-sequence B a Q-*choice* of A iff B_j is a choice set of $(A \setminus < \bigcup_{0 \leq k < j} B_k >^{A}_{j,Q_j})/Q_j$ for all $0 \leq j < i$, B a *full Q-choice* of A iff B is a Q-choice of A and $i = m$ and, finally $\bigcup \mathrm{rg}(B)$ a Q-*contraction* of A, for any full Q-choice B of A.

Until Proposition 1.4 let $m \in \mathbb{N}$, Q be an increasing m-sequence of equivalence relations over A, $B \subseteq A$, $0 \le i \le m$ and the i-sequence C be a Q-choice of B.

Proposition 1.2

(a) *Assume that there is an injective F from B to A with $Q_0(F(a), a)$ for all $a \in B$. Then $(F(C_j))_{0 \le j < i}$ is a Q-choice of $F(B)$.*

(b) *Assume that $\bigcup \mathrm{rg}(C) \subseteq E \subseteq B$. Then C is a Q-choice of E.*

(c) *For all $a \in B$ and all $0 \le j < i$ all or $> j$ elements $b \in B$ having Q_j with a are in $\bigcup_{0 \le k \le j} C_k$.*

(d) *For all $a \in A$ the number of elements in $\bigcup \mathrm{rg}(C)$ having Q_0 with a is $\le i$.*

(e)

$$|\bigcup \mathrm{rg}(C)| \le \sum_{j=0}^{i} |B/Q_j| \le i|B/Q_0|.$$

(f) *Let $\bar{Q}$ be an increasing m-sequence of equivalence relations over B such that Q_j is finer than $\bar{Q}_j$ for all $0 \le j < m$. For some i-sequence D that is a $\bar{Q}$-choice of B we have that $D_j \subseteq C_j$ for all $0 \le j < i$.*

Proof. These six statements can be easily proven by induction on the length i of the sequence. $\diamondsuit$

Proposition 1.3 *Let $B \subseteq E \subseteq A$ and the i-sequence D be a Q-choice of E. There is an injective $F \colon \bigcup \mathrm{rg}(C) \to \bigcup \mathrm{rg}(D)$ such that $Q_j(F(a), a)$ and $F(C_j) \subseteq \bigcup_{0 \le k \le j} D_k$ for all $0 \le j < i$ and all $a \in C_j$.*

Proof. The claim holds for $i = 0$. In the induction step assume it holds for $i = n$. We show its validity for $i = n + 1$. By induction hypothesis there is an injective $G : \bigcup_{0 \le j < n} C_j \to \bigcup_{0 \le j < n} D_j$ such that $Q_j(G(a), a)$ and $G(C_j) \subseteq \bigcup_{0 \le k \le j} D_k$ for all $0 \le j < n$ and all $a \in C_j$. We extend G to a function F as in the thesis. Assume $a \in C_n$. Then $a \in B \setminus \bigcup_{0 \le j < n} C_j$ and there are $k \le n$ elements in $\bigcup_{0 \le j < n} C_j$ having Q_n with a. Because of G there are $\bar{k} \ge k$ elements in $\bigcup_{0 \le j < n} D_j$ having Q_n with a. If $\bar{k} > k$, there is $b \in \bigcup_{0 \le j < n} D_j \setminus \mathrm{rg}(G)$ with $Q_n(a, b)$ and we set $F(a) = b$. If $\bar{k} = k$, there is $b \in E \setminus \bigcup_{0 \le j < n} D_j$ with $Q_n(a, b)$, whence $c \in D_n$ with $Q_n(a, c)$ and we set $F(a) = c$. Since C_n is a choice set of a set of equivalence classes of Q_n, F is injective. $\diamondsuit$

Corollary 1.1 *Let the i-sequence D be a Q-choice of B. There is a bijection $F : \bigcup \mathrm{rg}(C) \to \bigcup \mathrm{rg}(D)$ such that $Q_j(F(a), a)$ and $F(C_j) = D_j$ for all $0 \le j < i$ and all $a \in C_j$.*

Proof. By Proposition 1.3, since $B \subseteq B$, there is an injective $F : \bigcup \mathrm{rg}(C) \to \bigcup \mathrm{rg}(D)$ such that $Q_j(F(a), a)$ and $F(C_j) \subseteq \bigcup_{0 \le k \le j} D_k$ for all $0 \le j < i$ and all $a \in C_j$ and an injective $G : \bigcup \mathrm{rg}(D) \to \bigcup \mathrm{rg}(C)$ such that $Q_j(G(a), a)$ and $G(D_j) \subseteq \bigcup_{0 \le k \le j} C_k$ for all $0 \le j < i$ and all $a \in D_j$. By induction, assume $F(C_k) = D_k$ and $G(D_k) = C_k$ for all $0 \le k < j < i$. Then $F(C_j) \subseteq D_j$ and, since the elements of C_j pairwise do not have Q_j, $G \circ F\,(C_j) = C_j$. Therefore $F(C_j) = D_j$ and $G(D_j) = C_j$. $\diamondsuit$

Corollary 1.2 *Any two Q-contractions of B have the same cardinality.*

Proof. Immediate. $\diamondsuit$

Corollary 1.3 *Assume that $i > 0$ and that the i-sequence D is a Q-choice of B. Then there is a bijection F from B to B with $F(\bigcup \mathrm{rg}(C)) = \bigcup \mathrm{rg}(D)$ and $Q_{i-1}(F(a), a)$ for all $a \in B$.*

Proof. Left to the reader. ◇

Corollary 1.4 *Let the i-sequence D be a Q-choice of $\bigcup \mathrm{rg}(C)$. $\bigcup \mathrm{rg}(C) = \bigcup \mathrm{rg}(D)$.*

Proof. By Proposition 1.2 (b) C is a Q-choice of $\bigcup \mathrm{rg}(C)$. By Corollary 1.3 there is a bijection F from $\bigcup \mathrm{rg}(C)$ to $\bigcup \mathrm{rg}(C)$ with $F(\bigcup \mathrm{rg}(C)) = \bigcup \mathrm{rg}(D)$, whence $\bigcup \mathrm{rg}(C) = \bigcup \mathrm{rg}(D)$. ◇

Corollary 1.5 *Let D be a Q-contraction of B. $D = E$ for every Q-contraction E of D.*

Proof. Immediate from Corollary 1.4. ◇

The converse of Corollary 1.1 is true, too.

Proposition 1.4 *If F is an injective function from $\bigcup \mathrm{rg}(C)$ to B such that $Q_j(F(a), a)$ for all $0 \leq j < i$ and all $a \in C_j$, then $(F(C_j))_{0 \leq j < i}$ is a Q-choice of B.*

Proof. Induction over i. ◇

Let again $m \in \mathbb{N}$, $0 \leq i \leq m$ and Q respectively R be an increasing m- respectively i-sequence of equivalence relations over the set A such that Q_j is finer than R_j $(0 \leq j < i)$.

Corollary 1.6 *Every Q-contraction of A includes an R-contraction of A.*

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2 n-multigraphs

Chapter 2 introduces and examines n-multigraphs, which are the structures that essentially this book is about, under the aspects that are relevant for this work: the degree and the neighbourhood of their points. The results presented in this chapter belong to, or straightforwardly follow from, the ground knowledge in graph theory and topology. For this reason the proofs are often kept short and sometimes omitted. These results will be used for showing both the solvability and the unsolvability of the problems in the later chapters.

The *multigraph symbols*, that will also be used in later chapters, are the 2-placed relation symbols $R_1, R_2, \ldots$ (indeed, $R_i \neq R_j$ for $i \neq j$). Let $n \in \mathbb{N}$. S_n denotes the set $\{R_1, \ldots, R_n\}$ (of multigraph symbols) and T_n the first-order theory in S_n:

$$\{\, \forall xy \bigwedge_{1 \leq i < j \leq n} (R_i xy \to \neg R_j xy), \;\; \forall xy \bigwedge_{1 \leq i \leq n} (R_i xy \to R_i yx) \,\}.$$

An *n-multigraph* is a structure G over S_n satisfying the following two conditions:

(i) For all $a, b \in \mathrm{dom}(G)$ there is at most one $1 \leq i \leq n$ with $R_i^G(a, b)$. The *valence* (or *multiplicity*), $\mathrm{val}_G(a, b)$, of a, b in G is i, if $1 \leq i \leq n$ and $R_i^G(a, b)$; it is 0, if there is no $1 \leq i \leq n$ with $R_i^G(a, b)$.

(ii) Every R_i^G $(1 \leq i \leq n)$ is symmetric (over $\mathrm{dom}(G)$), i. e.

$$G \models \forall xy (R_i xy \to R_i yx).$$

Hence an n-multigraph is a structure over S_n that is a model of T_n. An n-multigraph G is called *m-bound* iff $\mathrm{val}_G(a,b) \leq m$ for all $a \neq b$ in $\mathrm{dom}(G)$ ($m \in \mathbb{N}$). Notice that a graph in the usual meaning is an irreflexive 1-multigraph.

2.1 Degree of an element

Let $n \in \mathbb{N}$. The *degree* of a in the n-multigraph G, $\deg_G(a)$, is defined by

$$\deg_G(a) = \begin{cases} \sum\limits_{\substack{b \in \mathrm{dom}(G)\setminus\{a\} \\ \mathrm{val}_G(a,b)\neq 0}} \mathrm{val}_G(a,b), & \text{if } \{b \in \mathrm{dom}(G) \mid \mathrm{val}_G(a,b) \neq 0\} \text{ is finite;} \\ \infty, & \text{otherwise;} \end{cases}$$

for all $a \in \mathrm{dom}(G)$. $\deg_G$ is regarded as a function whose domain is $\mathrm{dom}(G)$. G is said to be of *finite degree* iff $\deg_G(a) \neq \infty$ for every $a \in \mathrm{dom}(G)$. G is of *degree* k iff k is the highest degree in G of an element of $\mathrm{dom}(G)$ (∞ is by definition greater than any $n \in \mathbb{N}$). The n-multigraphs G, H are said to be *similar* iff they have the same domain and for all $a \in \mathrm{dom}(G)$

$\deg_G(a) = \deg_H(a)$ and $\mathrm{val}_G(a,a) = \mathrm{val}_H(a,a)$.

$d\colon A \to \{0,\ldots,n\}$ is called a *degree function* iff $A = \emptyset$ or there is an n-multigraph G with $\deg_G = d$. Notice that if $d\colon A \to \{0,\ldots,m\}$ ($m \in \mathbb{N}$), then there is an n-multigraph G with $\deg_G = d$ iff there is an m-multigraph G with $\deg_G = d$.

Suppose that $d\colon A \to \{0,\ldots,n\}$ for some finite set $A \neq \emptyset$ and set

$$\Delta = \Big(\sum_{b \in A\setminus\{a\}} d(b)\Big) - d(a)$$

with $a \in A$ such that $d(a) \geq d(b)$ for all $b \in A$.

$$\wedge((x \neq y \neq z \neq w \neq x \neq z \wedge y \neq w \wedge R_1xy \wedge R_1xz) \to \textstyle\bigwedge_{1\leq i\leq n} \neg R_ixw)).$$

Let $\Omega_i^n(x)$ $(n, i \in \mathbb{N})$ be an existential formula in S_n with i quantifiers such that

$$G \models \Omega_i^n[a] \text{ iff } \deg_G(a) \geq i$$

for all n-multigraphs G and all $a \in \mathrm{dom}(G)$.

Then the formula $\Xi_i^n = (\Theta_i^n \wedge \Omega_i^n)$ means in any n-multigraph G that x has degree i. Notice that Ξ_i^n is not the most economical way to express the above meaning. For example

$$\exists yz\forall w(x \neq y \wedge x \neq z \wedge ((y = z \wedge R_2xy) \vee ((y \neq z \wedge R_1xy \wedge R_1xz))$$

$$\wedge(y \neq w \neq z \to \textstyle\bigwedge_{1\leq i\leq n} \neg R_ixw))$$

is equivalent in every n-multigraph $(n \geq 2)$ to Ξ_2^n.

For $d\colon \{0, \ldots, n\} \to \mathbb{N}$ let T_d be the theory

$$\mathrm{T}_n \cup \{\forall x(R_ixx \to \Xi_{d(i)}^n) \mid 0 < i \leq n\} \cup \{\forall x(\bigwedge_{1\leq i\leq n} \neg R_ixx \to \Xi_{d(0)}^n)\}.$$

Then T_d axiomatizes the class of n-multigraphs with degree requirement d (i. e. the class of models of T_d over S_n is the class of n-multigraphs with degree requirement d).

2.2 Neighbourhoods

The *neighbourhood*, $\mathrm{nb}_G(A)$, of $A \subseteq \mathrm{dom}(G)$ in the n-multigraph G is the set

$$A \cup \{b \in \mathrm{dom}\,(G) \mid \text{ there is } a \in A \text{ with } \mathrm{val}_G(a, b) \neq 0\}.$$

The *k-neighbourhood*, $\mathrm{nb}^k_G(A)$, and the *closure*, $\mathrm{cl}_G(A)$, of A in G are given by

$$\begin{aligned}
\mathrm{nb}^0_G(A) &= A;\\
\mathrm{nb}^{(k+1)}_G(A) &= \mathrm{nb}_G(\mathrm{nb}^k_G(A)).\\
\mathrm{cl}_G(A) &= \bigcup\,\{\mathrm{nb}^k_G(A) \mid k \in \mathbb{N}\}.
\end{aligned}$$

Disregarding the risk of ambiguity, $\mathrm{nb}_G(A)$, $\mathrm{nb}^k_G(A)$ and $\mathrm{cl}_G(A)$ are simply written $\mathrm{nb}_G(a)$, $\mathrm{nb}^k_G(a)$ and $\mathrm{cl}_G(a)$ for $A = \{a\}$. A *component* of G is the closure $\mathrm{cl}_G(a)$ in G of an element $a \in \mathrm{dom}(G)$. Obviously $\mathrm{nb}_G(A) = \mathrm{nb}^1_G(A)$.

Proposition 2.3 (a) $\mathrm{nb}^k_G(A) = \bigcup\{\mathrm{nb}^k_G(a) \mid a \in A\}$ $(A \subseteq \mathrm{dom}(G))$.

(b) $\mathrm{nb}^k_G(\bigcup \mathcal{A}) = \bigcup\{\mathrm{nb}^k_G(A) \mid A \in \mathcal{A}\}$ *for every set* $\mathcal{A}$ *of subsets of* $\mathrm{dom}(G)$.

(c) *For all* $a, b \in \mathrm{dom}(G)$

$$a \in \mathrm{nb}^k_G(b) \textit{ iff } b \in \mathrm{nb}^k_G(a).$$

Proof. (a) can be verified by induction. (b) is a set theoretical consequence of (a). (c) It suffices to prove that if $a \in \mathrm{nb}^k_G(b)$, then $b \in \mathrm{nb}^k_G(a)$. It is straightforward to shown that the following two statements hold:

(1) $a \in \mathrm{nb}_G(b)$ iff $b \in \mathrm{nb}_G(a)$.

(2) $\mathrm{nb}_G(\mathrm{nb}^k_G(A)) = \mathrm{nb}^k_G(\mathrm{nb}_G(A))$ $(A \subseteq \mathrm{dom}(G))$.

Now the prove is by induction, the case $k = 0$ being immediate. For the induction step let $a \in \mathrm{nb}^{k+1}_G(b)$. Then $a \in \mathrm{nb}_G(c)$ for some $c \in \mathrm{nb}^k_G(b)$. By induction hypothesis and by (1), $b \in \mathrm{nb}^k_G(c)$ for some $c \in \mathrm{nb}_G(a)$. Using (a) we obtain $b \in \mathrm{nb}^k_G(\mathrm{nb}_G(a))$. Now (2) yields $b \in \mathrm{nb}^{k+1}_G(a)$. $\diamondsuit$

Proposition 2.8 *Suppose* $A \subseteq \mathrm{dom}(H)$ *and* $\deg_G(a) \in \mathbb{N}$ *for all* $a \in A$. *Then* $\deg_G(a) = \deg_H(a)$ *for all* $a \in A$ *iff* $\mathrm{nb}_G(A) = \mathrm{nb}_H(A)$.

Proof. $\Leftarrow$. Since $\deg_K(b) = \deg_{K|\ \mathrm{nb}_K(B)}(b)$ for all n-multigraphs K, $B \subseteq \mathrm{dom}(K)$ and $b \in B$, the right side implies the left one. $\Rightarrow$. Suppose $\deg_G(a) = \deg_H(a)$ for all $a \in A$. For all $a \in A$

$$\deg_G(a) = \deg_H(a) \ + \sum_{\substack{b \in \mathrm{dom}(G) \setminus \mathrm{dom}(H) \\ \mathrm{val}_G(a,b) \neq 0}} \mathrm{val}_G(a,b).$$

Hence the right summand is 0. This equality implies $\mathrm{nb}_G(A) \subseteq \mathrm{dom}(H)$. Proposition 2.6(b) yields $\mathrm{nb}_G(A) = \mathrm{nb}_H(A)$. ♢

2.3 Closed subsets

Let G be an n-multigraph and $A \subseteq \mathrm{dom}(G)$. A is said to be *k-closed* in G iff $\mathrm{cl}_G(A) = \mathrm{nb}_G^k(A)$ and *closed* in G iff it is 0-closed in G (i. e. $\mathrm{cl}_G(A) = A$). H is a *closed substructure* of G iff $H \subseteq G$ and $\mathrm{dom}(H)$ is closed in G. The following proposition is easy to prove.

Proposition 2.9 *A is closed in G iff* $\mathrm{nb}_G(A) = A$. ♢

Proposition 2.9 implies that the definition of closed subset in this section is consistent with the definition given in Chapter 1, referring to arbitrary structures over sets of relation symbols.

From Proposition 2.9 and 2.3(b) it follows easily that $\mathrm{cl}_G(A)$ ($A \subseteq \mathrm{dom}(G)$) is closed in G and, from Corollary 2.1(a), that it is the smallest (with respect to $\subseteq$) $B \subseteq \mathrm{dom}(G)$

closed in G, containing A. Proposition 2.4(b) yields now that the components of G are precisely the minimal non-empty subsets of $\mathrm{dom}(G)$ closed in G. The next proposition is given without proof.

Proposition 2.10 *A set is closed in G iff it is a closed (or open) set in the topology for which the set of all components of G is a basis.* $\diamondsuit$

Proposition 2.11 *Suppose that $\deg_G(a) \in \mathbb{N}$ for all $a \in A$. A is closed in G iff $\deg_{G|A}(a) = \deg_G(a)$ for all $a \in A$.*

Proof. Easy with Proposition 2.9 and 2.8, given that $\mathrm{nb}_{G|A}(A) = A$. $\diamondsuit$

Let again G be an n-multigraph and $B \subseteq A \subseteq \mathrm{dom}(G)$. Proposition 2.11 implies the next corollary.

Corollary 2.2 *If $d\colon \{0, \ldots, n\} \to \mathbb{N}$, H is an n-multigraph and G, H have both degree requirement d, then $H \subseteq G$ iff H is a closed substructure of G.* $\diamondsuit$

Proposition 2.12 *Assume that A is closed in G and B is closed in $G|A$. Then B is closed in G.*

Proof. By Proposition 2.9 and 2.6(a) $\mathrm{nb}_G(B) \subseteq \mathrm{nb}_G(A) = A$. Therefore, with Proposition 2.5 and 2.9, $\mathrm{nb}_G(B) = \mathrm{nb}_G(B) \cap A = \mathrm{nb}_{G|A}(B) = B$. Hence, again by Proposition 2.9, B is closed in G. $\diamondsuit$

We will be interested in knowing whether there is an n-multigraph H similar to G in which A is closed. Obviously, from Proposition 2.9, if $\deg_G(a) \leq n$ for all $a \in \mathrm{dom}(G)$, this is the case iff both $\deg_G|A$ and $\deg_G|\,(\mathrm{dom}(G) \setminus A)$ are degree functions. Moreover, if G is finite and $\deg_G|A$ is a degree function, $\sum_{a \in \mathrm{dom}(G) \setminus A} \deg_G(a)$ is even. Hence we obtain from Proposition 2.1:

Corollary 2.3 *If G is finite of degree $\leq n$, $\deg_G|A$ is a degree function and*

$$|\,\{a \in \mathrm{dom}(G) \setminus A \mid \deg_G(a) \geq 1\}\,| > n,$$

then there is an n-multigraph H similar to G in which A is closed. $\diamondsuit$

2.4 Connected n-multigraphs

An n-multigraph is called *connected* iff it has exactly one component. That component A must be the domain, for, if there would be $a \notin A$ in the domain, its closure would be different from A. Let G be an n-multigraph. We can immediately conclude that, if G is connected, $\mathrm{cl}_G(a) = \mathrm{dom}(G)$ for all $a \in \mathrm{dom}(G)$.

Proposition 2.13 *G is connected iff $\mathrm{cl}_G(a) = \mathrm{dom}(G)$ for some $a \in \mathrm{dom}(G)$.*

Proof. $\Rightarrow$ follows directly from the conclusion above. $\Leftarrow$ follows easily from Proposition 2.4(b). $\diamondsuit$

Proposition 2.14 *The restriction of G to any of its component is connected.*

Proof. Let $a \in \mathrm{dom}(G)$ and set $H = G|\mathrm{cl}_G(a)$. By Corollary 2.1(b) with $A = B = \{a\}$, $\mathrm{dom}(H) = \mathrm{cl}_G(a) = \mathrm{cl}_H(a)$. With Proposition 2.13 H is connected. $\diamondsuit$

Proposition 2.18 *There is $a \in A \setminus B$ for which $H' = G|(B \cup \{a\})$ is connected. Therefore there is an injective $|A|$-sequence u to A for which $G|\{u_i \mid i < k\}$ is connected for all $0 < k \leq |A|$.*

Proof. There is $a \in A \setminus B$ with $a \in \mathrm{nb}_{G}(B)$, otherwise both B and $A \setminus B$ would be closed in G, by Proposition 2.9, contradicting the connectivity of G, since, given the discussion following Proposition 2.9, they would each include a component. Because H is finite and connected, there are $k \in \mathbb{N}, b \in B$ with $B = \mathrm{cl}_{H}(b) = \mathrm{nb}^{k}_{H}(b)$. Therefore $\mathrm{dom}(H') = \mathrm{nb}^{k+1}_{H'}(b) = \mathrm{cl}_{H'}(b)$. ♢

2.5 Gaifman graph and sum of structures

Let U be a structure over a set L of relation symbols. The *Gaifman graph* $\mathrm{gf}(U)$ of U is the 1-multigraph with domain $\mathrm{dom}(U)$ and in which R_1 holds exactly for all (a, b) with $a \neq b$ for which there are $R \in \mathrm{L}$ and $u_0, \ldots, u_{\nu_R - 1} \in \mathrm{dom}(U)$ such that $R^U(u_0, \ldots, u_{\nu_R-1})$ and $a, b \in \{u_0, \ldots, u_{\nu_R-1}\}$. The Gaifman graph of a structure is obviously a graph in the usual meaning. For $u \in \mathrm{dom}(U)$ we define $\deg_{U}(u) = \deg_{\mathrm{gf}(U)}(u)$. U is of *finite degree* iff $\mathrm{gf}(U)$ is of finite degree. A *component* of U is a component of $\mathrm{gf}(U)$. U is called *connected* iff $\mathrm{gf}(U)$ is connected. The following two propositions are immediate.

Proposition 2.19 *If $V \subseteq U$, then $\mathrm{id}_{\mathrm{dom}(V)}$ is a homomorphism from $\mathrm{gf}(V)$ to $\mathrm{gf}(U)$.* ♢

Proposition 2.20 *$A \subseteq \mathrm{dom}(U)$ is closed in U iff it is closed in $\mathrm{gf}(U)$.* ♢

Proposition 2.21 (a) *Assume that* $V \subseteq U$ *and* $\mathrm{dom}(V)$ *is closed in* U. *Then* $\mathrm{gf}(V) = \mathrm{gf}(U)|\mathrm{dom}(V)$.

(b) *Assume that* $V \subseteq U$ *and every symbol in* L *is 1- or 2-placed. Then* $\mathrm{gf}(V) = \mathrm{gf}(U)|\mathrm{dom}(V)$.

(c) *If* V *is connected and* $V \subseteq U$, *then* $H := \mathrm{gf}(U)|\mathrm{dom}(V)$ *is connected.*

(d) *Let* $j, k \in \mathbb{N}$, $j \leq k$, $A \subseteq \mathrm{dom}(U)$ *and* $V = U|\mathrm{nb}^k_{\mathrm{gf}(U)}(A)$. $\mathrm{nb}^j_{\mathrm{gf}(U)}(A) = \mathrm{nb}^j_{\mathrm{gf}(V)}(A)$.

(e) *If* $W \subseteq U$ *is connected, then* $V := U|\mathrm{nb}_{\mathrm{gf}(U)}(\mathrm{dom}(W))$ *is connected.*

Proof. (a) Suppose $a, b \in \mathrm{dom}(V)$ and $R_1^{\mathrm{gf}(U)}(a, b)$. Then there are $R \in \mathrm{L}$ and $u_0, \ldots, u_{\nu_R - 1} \in \mathrm{dom}(U)$ such that $R^U(u_0, \ldots, u_{\nu_R-1})$ and $a, b \in \{u_0, \ldots, u_{\nu_R-1}\}$. Since $\mathrm{dom}(V)$ is closed in $\mathrm{gf}(U)$, $u_0, \ldots, u_{\nu_R-1} \in \mathrm{dom}(V)$. Hence $R_1^{\mathrm{gf}(V)}(a, b)$.

(b) For all $a, b \in \mathrm{dom}(V)$

$$\begin{aligned} R_1^{\mathrm{gf}(V)}(a,b) \quad &\text{iff} \quad a \neq b \text{ and } Q^V(a,b) \text{ or } Q^V(b,a) \text{ for a 2-placed relation symbol } Q \in \mathrm{L} \\ &\text{iff} \quad a \neq b \text{ and } Q^U(a,b) \text{ or } Q^U(b,a) \text{ for a 2-placed relation symbol } Q \in \mathrm{L} \\ &\text{iff} \quad R_1^{\mathrm{gf}(U)}(a,b). \end{aligned}$$

(c) There is $c \in \mathrm{dom}(V)$ with $\mathrm{dom}(V) = \mathrm{cl}_{\mathrm{gf}(V)}(c)$ and for all $a, b \in \mathrm{dom}(V)$ we have $R_1^H(a, b)$, if $R_1{}^{\mathrm{gf}(V)}(a, b)$. With Proposition 2.7 $\mathrm{dom}(V) = \mathrm{cl}_{\mathrm{gf}(V)}(c) \subseteq \mathrm{cl}_H(c) \subseteq \mathrm{dom}(V)$.

(d) Since $V \subseteq U$, by Proposition 2.19 and Proposition 2.7, $\mathrm{nb}^j_{\mathrm{gf}(V)}(A) \subseteq \mathrm{nb}^j_{\mathrm{gf}(U)}(A)$. We show by induction on j that $\mathrm{nb}^j_{\mathrm{gf}(U)}(A) \subseteq \mathrm{nb}^j_{\mathrm{gf}(V)}(A)$. The claim clearly holds for $j = 0$. Assume it holds for $j < k$ and let $v \in \mathrm{nb}^{j+1}_{\mathrm{gf}(U)}(A) \setminus \mathrm{nb}^j_{\mathrm{gf}(U)}(A)$. Then there is for all structures U and all $u \in \mathrm{dom}(U)$. Then the formula $\Xi_i^L = (\Theta_i^L \wedge \Omega_i^L)$ means in any structure U over L that x has degree i.

Let $\mathcal{U}$ a set of connected structures over L of cardinality at most l. If $\mathcal{U} = \emptyset$, set $\vartheta_{\mathcal{U}}$ to be the false sentence. If $\mathcal{U} \neq \emptyset$, let U be a combination of $\mathcal{U}$ such that for every $V \in \mathcal{U}$ there are precisely l components A of U with $U|A \cong V$ and set

$$\vartheta_{\mathcal{U}} = \forall x_0 \dots x_{l+m-1} \bigvee_{u=u_0,\dots,u_{l+m-1} \in \mathrm{dom}(U)} (\Delta_{U,u} \wedge \Xi^L_{\mathrm{deg}_U(u_0)}(x_0) \wedge \dots \wedge \Xi^L_{\mathrm{deg}_U(u_{l-1})}(x_{l-1})).$$

Proposition 2.30 *$\vartheta_{\mathcal{U}}$ is logically equivalent to a universal-existential sentence and axiomatizes the class of all combinations of $\mathcal{U}$.*

Proof. For any structure U over L we have

$V \models \vartheta_{\mathcal{U}}$ iff

for every at most l-element $W \subseteq V$ there is an embedding f of W into U with $\mathrm{deg}_V(v) = \mathrm{deg}_U(f(v))$ for all $v \in \mathrm{dom}(W)$ iff (by Corollary 2.4)

every restriction of V to a component is isomorphic to the restriction of U to a component iff

V is a combination of $\mathcal{U}$. $\diamondsuit$

2.6 A-homomorphisms

Let G, H be n-multigraphs and $A \subseteq \mathrm{dom}(G)$. A *weak A-homomorphism* from G to H is a homomorphism f from $G|\mathrm{nb}_G(A)$ to H such that $f(\mathrm{nb}_G(u)) = \mathrm{nb}_H(f(u))$ for all $u \in A$. Assume that f is a weak A-homomorphism from G to H and $u \in A$ with $\deg_G(u) = \deg_H(f(u))$.

Proposition 2.31 *$f|\mathrm{nb}_G(u)$ is injective.*

Proof. Let $\{b_0, \ldots, b_{i-1}\} = \mathrm{nb}_H(f(u)) \setminus \{f(u)\}$ and $b_0, \ldots, b_{i-1}$ distinct. There are distinct $a_0, \ldots, a_{i-1} \in \mathrm{nb}_G(u) \setminus \{u\}$ with $f(a_j) = b_j$ $(0 \leq j < i)$. We have $\deg_H(f(u)) = \sum_{0 \leq j < i} \mathrm{val}_H(f(u), b_j) = \sum_{0 \leq j < i} \mathrm{val}_G(u, a_j)$. Therefore

$$\deg_G(u) = \deg_H(f(u)) + \sum_{v \in \mathrm{nb}_G(u) \setminus \{a_0, \ldots, a_{i-1}, u\}} \mathrm{val}_G(u, v).$$

Since $\deg_H(f(u)) = \deg_G(u)$, we have

$$\sum_{v \in \mathrm{nb}_G(u) \setminus \{a_0, \ldots, a_{i-1}, u\}} \mathrm{val}_G(u, v) = 0.$$

Hence $\{a_0, \ldots, a_{i-1}, u\} = \mathrm{nb}_G(u)$. $\diamondsuit$

An *A-homomorphism* from G to H is a weak A-homomorphism f from G to H for which $f|A$ is a partial isomorphism from G to H. Let f be an A-homomorphism from G to H and G, H have degree requirement $d \colon \{0, \ldots, n\} \to \mathbb{N}$.

Corollary 2.5 *Let $a, b \in A$, $c \in \mathrm{nb}_G(a)$, $d \in \mathrm{nb}_G(b)$. Suppose $f(a) = f(b)$ and $f(c) = f(d)$. Then $a = b$ and $c = d$.*

Proof. $a = b$, because $f|A$ is a partial isomorphism. Therefore $c, d \in \mathrm{nb}_G(a)$. Proposition 2.31 implies $c = d$. $\diamondsuit$

Proposition 2.32 *Let $a \in \mathrm{nb}_G(A) \setminus A$. Then $f(a) \notin f(A)$.*

H_{i+1} is a 1-fold shift of H_i ($0 \leq i < k$). This means that H is synthesizable from G iff H is a shift of G (i. e. a k-fold shift of G for some $k \in \mathbb{N}$).

Let $n \in \mathbb{N}$, G, H be n-multigraphs and $\mathcal{S}$ be a set of n-rules.

Proposition 3.4 *If H is $\mathcal{S}$-synthesizable (in k steps) from G and $G \subseteq \bar{G}$, then the $\bar{G}$-extension of H by $\mathrm{id}_{\mathrm{dom}(G)}$ is $\mathcal{S}$-synthesizable (in k steps) from $\bar{G}$. Therefore, if H is an (k-step) $\mathcal{S}$-product of G, then H is an (k-step) $\mathcal{S}$-product of any extension of G.*

Proof. Since $\mathrm{sh}(\bar{G}, a)$ is the $\bar{G}$-extension of $\mathrm{sh}(G, a)$ by $\mathrm{id}_{\mathrm{dom}(G)}$, if $G \subseteq \bar{G}$ and a is a $4k$-sequence to $\mathrm{dom}(G)$, the proof is immediate from the definition of $\mathcal{S}$-shift and $\mathcal{S}$-product. $\diamondsuit$

Corollary 3.1 *Let $\mathcal{G}$ be a set of n-multigraphs with pairwise disjoint domains. H is an (k-step) $\mathcal{S}$-product of a combination of $\mathcal{G}$ iff it is an (k-step) $\mathcal{S}$-product of a combination of $\sum \mathcal{G}$. If $\mathcal{G}$ is finite, then H is an (k-step) $\mathcal{S}$-product of a finite-combination of $\mathcal{G}$ iff it is an (k-step) $\mathcal{S}$-product of a finite-combination of $\sum \mathcal{G}$.*

Proof. Every combination of $\sum \mathcal{G}$ is a combination of $\mathcal{G}$ and, if $\mathcal{G}$ is finite, every finite-combination of $\sum \mathcal{G}$ is a finite-combination of $\mathcal{G}$. Assume that H is an (k-step) $\mathcal{S}$-product of a (finite-)combination of $\mathcal{G}$. Then there is a (finite) combination set $\mathcal{H}$ of $\mathcal{G}$ such that H is an (k-step) $\mathcal{S}$-product of $\sum \mathcal{H}$. Let $\mathcal{K}$ be a combination set of $\sum \mathcal{G}$ with cardinality $|\mathcal{H}|$. Obviously, $\sum \mathcal{K}$ extends a structure K isomorphic to $\sum \mathcal{H}$. A structure H_0, isomorphic to H, is an (k-step) $\mathcal{S}$-product of K. By Proposition 3.4 H_0 is

Proof. The two directions of the implication are proven by induction, $\Rightarrow$ on l, $\Leftarrow$ on the length of the synthesis. For $\Leftarrow$ note that G is an $\mathcal{S}$-shift of G for any n-multigraph G, since $\mathcal{S}\text{-sh}(G, \emptyset) = G$. $\diamondsuit$

We now take a look at the n-rules from a graph theoretical perspective.

Proposition 3.7 *Let* (K, u) *be a 1-fold* n*-rule,* $G = \text{sh}(K, u)$ *and* $C = cl_K(u_0) \cup cl_K(u_2)$*.* $G = \text{sh}(K|C, u) \oplus K|(\text{dom}(K) \setminus C)$ *and* $C = \text{cl}_G(u_0) \cup \text{cl}_G(u_2)$*.*

Proof. Since C is closed in K and $u_0, u_1, u_2, u_3 \in C$, $G = \text{sh}(K|C, u) \oplus K|(\text{dom}(K) \setminus C)$.

We prove that $C = \text{cl}_G(u_0) \cup \text{cl}_G(u_2)$. Define $C_i = C \setminus \{u_j \,|\, 0 \leq j < 4 \text{ and } j \neq i\}$ and $K_i = K|C_i$ $(0 \leq i < 4)$. Then $K_i = G|C_i$ $(0 \leq i < 4)$. For every $b \in C$ there are $0 \leq i < 4$ and $k \in \mathbb{N}$ such that $b \in \text{nb}^k_K(u_i)$ and k is the smallest $j \in \mathbb{N}$ with $b \in \text{nb}^j_K(u_m)$ for some $0 \leq m < 4$. The proof, by induction, that $b \in \text{nb}^k_{K_i}(u_i)$ is left to the reader. $K_i = G|C_i$ $(0 \leq i < 4)$ implies $b \in \text{cl}_G(\{u_0, u_1, u_2, u_3\})$. Since $\text{cl}_G(u_0) = \text{cl}_G(u_3)$ and $\text{cl}_G(u_2) = \text{cl}_G(u_1)$, $C = \text{cl}_G(u_0) \cup \text{cl}_G(u_2)$. $\diamondsuit$

A k-fold n-rule (K, u) is called *unfragmented* iff $\text{dom}(K) = \text{cl}_K(\{u_0, \ldots, u_{4k-1}\})$.

Corollary 3.2 *Let* $\mathcal{S}$ *be a set of 1-fold, unfragmented* n*-rules and* $G_0, \ldots, G_l$ *an* $\mathcal{S}$*-synthesis. Assume that* $C \subseteq \text{dom}(G_0)$ *is closed in every* G_i $(0 \leq i \leq l)$*. Then* $G_0|C, \ldots, G_l|C$ *is an* $\mathcal{S}$*-synthesis.*

Proof Suppose the thesis does not hold. By Proposition 3.7 there are $0 \leq i \leq l$ and a 4-sequence u to $\text{dom}(G_i)$ such that $G_{i+1} = \text{sh}(G_i, u)$, $G_{i+1} \neq G_i$ and $u_0 \in C, u_2 \notin C$ or

$u_0 \notin C, u_2 \in C$. Since C is closed in G_i, we have that $u_1 \in C, u_2 \notin C$ or $u_1 \notin C, u_2 \in C$. But $u_1 \in \mathrm{nb}_{G_{i+1}}(u_2)$, contradicting that C is closed in G_{i+1}. $\diamondsuit$

Next we proceed with some important classifications of the n-rules based on their graph theoretical properties. An *n-addition* is an unfragmented, k-fold n-rule (K, u) with $u_{4i+2} \notin \mathrm{cl}_{\mathrm{sh}(K,u_0,\ldots,u_{4i-1})}(u_{4i+1})$ for all $0 \leq i < k$.

Proposition 3.8 *If (K, u) is a 1-fold n-addition and the 4-sequence v to* $\mathrm{dom}(K)$ *is equivalent in K to u, then (K, v) is an n-addition, too.* $\diamondsuit$

An n-rule is an *n-elimination* iff its inverse is an n-addition. Therefore, a k-fold n-rule (K, u) is an n-elimination iff it is unfragmented and $u_{4i+3} \notin \mathrm{cl}_{\mathrm{sh}(K,u_0,\ldots,u_{4i+3})}(u_{4i+2})$ for all $0 \leq i < k$. In the language of graph theory an n-elimination is an unfragmented n-rule (K, u) such that the set $\{\{u_{4i}, u_{4i+1}\}, \{u_{4i+2}, u_{4i+3}\}\}$ of edges separates $\{u_{4i}, u_{4i+3}\}$ and $\{u_{4i+1}, u_{4i+2}\}$ in $\mathrm{gf}(\mathrm{sh}(K, u_0, \ldots, u_{4i-1}))$ and $\mathrm{val}_{\mathrm{sh}(K,u_0,\ldots,u_{4i+3})}(u_{4i}, u_{4i+1})$ $= \mathrm{val}_{\mathrm{sh}(K,u_0,\ldots,u_{4i-1})}(u_{4i+2}, u_{4i+3}) = 1$ $(0 \leq i < k)$.

An n-rule that is both an n-addition and an n-elimination is called an *n-substitution*. A k-fold n-rule (K, u) is called *building* respectively *separating* iff $(\mathrm{sh}(K, u_0, \ldots, u_{4i-1}),$ $u_{4i}, u_{4i+1}, u_{4i+2}, u_{4i+3})$ is not an n-elimination respectively not an n-addition for all $0 \leq i < k$. It follows immediately that if (K, u) is building, its inverse is separating and vice versa.

Proposition 3.9 *A 1-fold n-rule (K, u) is an n-addition iff there are $a, b \in$* $\mathrm{dom}(K)$ *such that $a \notin \mathrm{cl}_K(b)$ but $a \in \mathrm{cl}_{\mathrm{sh}(K,u)}(b)$.*

Corollary 3.6 *If (K, u) is a building n-rule, every component of K is contained in a component of* $\mathrm{sh}(K, u)$. $\diamondsuit$

If (K, u) is a 1-fold, building n-rule and $G = \mathrm{sh}(K, u)$, $\mathrm{cl}_G(u_0) = \mathrm{cl}_G(u_2)$. Therefore Corollary 3.6 is also a corollary of Proposition 3.7.

Corollary 3.7 *If (K, u) is a separating n-rule, every component of* $\mathrm{sh}(K, u)$ *is contained in a component of K.* $\diamondsuit$

An $\mathcal{S}$-shift is defined on the ground of a set $\mathcal{S}$ of n-rules. We can increase the expressive power for the selection of the points at which the shift can be applied by using first-order formulas. Let $\zeta(x_0, \ldots, x_{4k-1})$ be a formula in S_n (for the sake of precision where x_{4k-1} occurs free, if $k > 0$). The *ζ-shift* of the n-multigraph G, ζ-$\mathrm{sh}(G, u)$, at the $4l$-sequence u to $\mathrm{dom}(G)$ is given by:

ζ-$\mathrm{sh}(G, u) = \mathrm{sh}(G, u)$, if $l = k$ and $G \models \zeta[u]$;

ζ-$\mathrm{sh}(G, u) = G$, otherwise.

A *ζ-shift* of G is a ζ-shift of G at some $4l$-sequence to $\mathrm{dom}(G)$. Let $\mathcal{S}$ be a finite set of finite k-fold n-rules,

$\zeta = \bigvee_{(K,u)\in\mathcal{S}} \exists x_{4k} \ldots \exists x_{4k+m_{K,u}-1} \Delta_{K,v_{K,u}}$, if $k > 0$ and

$\zeta = \exists x_0 x_0 \neq x_0$, if $k = 0$,

where $m_{K,u} = |\mathrm{dom}(K)| - |\{u_0, \ldots, u_{4k-1}\}|$ and $v_{K,u}$ is a surjective sequence u, a to $\mathrm{dom}(K)$ for some $m_{K,u}$-sequence a ($(K, u) \in \mathcal{S}$). ζ is a formula in S_n. x_{4k-1} occurs free in $\zeta(x_0, \ldots, x_{4k-1})$, if $k > 0$ and $\mathcal{S} \neq \emptyset$; ζ has no free variables, otherwise.

Proposition 3.10 *For all n-multigraphs G and all $4k$-sequences u to* $\mathrm{dom}(G)$

$$\mathcal{S}\text{-sh}(G,u) = \zeta\text{-sh}(G,u). \qquad \diamondsuit$$

On the other hand we have:

Proposition 3.11 *For every existential $\zeta(x_0,\ldots,x_{4k-1})$ in S_n, in which x_{4k-1} occurs free in φ, if $k > 0$, there is a finite set $\mathcal{S}$ of finite k-fold n-rules such that for all n-multigraphs G and all $4k$-sequences u to* $\mathrm{dom}(G)$

$$\mathcal{S}\text{-sh}(G,u) = \zeta\text{-sh}(G,u).$$

Proof. Let $\zeta = \exists x_{4k} \ldots \exists x_{4k+m-1}\xi$ with quantifier-free $\xi(x_0,\ldots,x_{4k+m-1})$. Write ξ as a disjunction of $(4k+m)$-types of S_n. $\diamondsuit$

3.2 Synthesizability problems

We denote by $\mathcal{G}$ the class of all structures that are finite n-multigraphs for some $n \in \mathbb{N}$ and by $\mathcal{R}$ the class of all sets that, for some $n \in \mathbb{N}$, are finite sets of finite n-rules.

If $\mathcal{C}_0, \mathcal{C}_1 \subseteq \mathcal{G}$ and $\mathcal{Q} \subseteq \mathcal{R}$ are decidable classes (closed under isomorphism[1]), the *(closed) $\mathcal{Q}$-synthesizability* problem for $\mathcal{C}_0, \mathcal{C}_1$ is the question:

> Given $n \in \mathbb{N}$, a set $\mathcal{S} \in \mathcal{Q}$ of n-rules, n-multigraphs $H \in \mathcal{C}_0$ and $G \in \mathcal{C}_1$, is G an (closed) $\mathcal{S}$-product of a combination of H?

[1] $\mathcal{S}, \mathcal{T} \in \mathcal{R}$ are *isomorphic* iff for some $n \in \mathbb{N}$ they are both sets of n-rules, for every $P \in \mathcal{S}$ there is a $Q \in \mathcal{T}$ with $P \cong Q$ and vice versa.

We omit $\mathcal{C}_1$ in the above definition, if $\mathcal{C}_1 = \mathcal{G}$. As usual, in spite of a possible ambiguity, when assigning a value to $\mathcal{C}_0, \mathcal{C}_1$ or $\mathcal{Q}$, we write $\mathcal{S}$ for the class of all $\mathcal{T} \in \mathcal{R}$ isomorphic to $\mathcal{S}$ and G for the class of all $H \in \mathcal{G}$ isomorphic to G. In the case that $\mathcal{C}_0$ is closed under finite combinations, by Corollary 3.1, the question can be rewritten:

> Given $n \in \mathbb{N}$, a set $\mathcal{S} \in \mathcal{Q}$ of n-rules, a finite set $\mathcal{H} \subseteq \mathcal{C}_0$ of n-multigraphs and an n-multigraph $G \in \mathcal{C}_1$, is G an (closed) $\mathcal{S}$-product of a combination of $\mathcal{H}$?

We now define the following classes:

$\mathcal{G}_d$ ($d\colon \{0, \dots, n\} \to \mathbb{N}$): class of all finite n-multigraphs with degree requirement d;

$\mathcal{G}_{\leq d}$ ($d : \{0, \dots, n\} \to \mathbb{N}$): class of all finite n-multigraphs G with $\deg_G(a) \leq d(\mathrm{val}_G(a, a))$ ($a \in \mathrm{dom}(G)$);

$\mathcal{G}^{\mathrm{dr}}$: class of all $G \in \mathcal{G}$ that for some $n \in \mathbb{N}$ are n-multigraphs with some degree requirement $d\colon \{0, \dots, n\} \to \mathbb{N}$;

$\mathcal{G}^{\mathrm{dd}}$: class of all $G \in \mathcal{G}$ that for some $n \in \mathbb{N}$ are n-multigraphs with some degree requirement $d\colon \{0, \dots, n\} \to \{0, \dots, n\}$;

$\mathcal{G}^{\mathrm{db}}$: class of all $G \in \mathcal{G}$ that for some $n \in \mathbb{N}$ are n-multigraphs with degree $\leq n$;

$\mathcal{G}^m$ ($m \in \mathbb{N}$): class of all m-bound $G \in \mathcal{G}$;

$\mathcal{G}^{\mathrm{conn}}$: class of all connected $G \in \mathcal{G}$;

$\mathcal{R}^m$ ($m \in \mathbb{N}$): class of all $\mathcal{S} \in \mathcal{R}$ that for some $n \in \mathbb{N}$ are a set of m-fold n-rules;

$\mathcal{R}^{\mathrm{a},m}$: class of all $\mathcal{S} \in \mathcal{R}$ that for some $n \in \mathbb{N}$ are a set of m-fold n-additions;

$\mathcal{R}^{\mathrm{ad}}$: class of all $\mathcal{S} \in \mathcal{R}$ that for some $n \in \mathbb{N}$ are a set of basic n-additions;

$\mathcal{R}^{\mathrm{vd}}$: class of all void $\mathcal{S} \in \mathcal{R}$;

$\mathcal{R}^{\mathrm{ub}}$: class of all $\mathcal{S} \in \mathcal{R}$ whose elements are 1-fold, unfragmented and building;

$\mathcal{R}^{\mathrm{sr}}$: class of all $\mathcal{S} \in \mathcal{R}$ whose elements are separating.

The following problems will be shown to be solvable:

the closed $\mathcal{R}^{\mathrm{ub}}$-synthesizability problem for $\mathcal{G}$;

the $\mathcal{R}^{\mathrm{sr}}$-synthesizability problem for $\mathcal{G}$;

the $\mathcal{R}^{\mathrm{ad}}$-synthesizability problem for $\mathcal{G}^{\mathrm{dr}}$, that will also be called *basic addition* problem;

the closed $\mathcal{R}^{\mathrm{ad}}$-synthesizability problem for $\mathcal{G}^{\mathrm{dr}}$ (as a direct consequence from the previous solvability);

the closed $\mathcal{R}^{\mathrm{vd}}$-synthesizability problem for $\mathcal{G}^{\mathrm{db}}$ and therefore for $\mathcal{G}^{\mathrm{dd}}$;

the $\mathcal{R}^{\mathrm{vd}}$-synthesizability problem for $\mathcal{G}^{\mathrm{db}}$ and therefore for $\mathcal{G}^{\mathrm{dd}}$ (we call the second one also *void synthesizability* problem).

At this point we introduce the function $d_n \colon \{0, \ldots, n\} \to \{1, 2\}$ ($n \geq 2$) that maps $0, 1, 2$ to 1 and $3, \ldots, n$ to 2.

The following problems will be shown to be unsolvable for a set $\mathcal{S}$ of at most 12-element, 2-fold 14-additions, a finite 14-multigraph H with degree requirement d_{14} and a 2-element 14-multigraph G, described in Section 5.2:

the $\mathcal{S}$-synthesizability problem and, consequently, the closed $\mathcal{S}$-synthesizability problem for H, $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1 \cap \mathcal{G}^{\mathrm{conn}}$;

the $\mathcal{S}$-synthesizability problem and, consequently, the closed $\mathcal{S}$-synthesizability problem for $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1, G$;

the $\mathcal{R}^{\mathrm{a},m}$-, $\mathcal{R}^m$-, closed $\mathcal{R}^{\mathrm{a},m}$- and closed $\mathcal{R}^m$-synthesizability problem for $\mathcal{G}^{\mathrm{dd}}$, if $m \geq 2$ (as an immediate consequence of any of the preceding unsolvabilities). The first two problems are more simply called *m-fold addition* respectively *m-fold synthesizability problem.*

Finally the following problems remain open with this book:

the $\mathcal{R}^1$-synthesizability problem for $\mathcal{G}^{\mathrm{dd}}$ (1-fold synthesizability problem);

the $\mathcal{R}^{\mathrm{a},1}$-synthesizability problem for $\mathcal{G}^{\mathrm{dd}}$ (1-fold addition problem) (in the case the preceding one is unsolvable).

3.3 The closed $\mathcal{R}^{\mathrm{ub}}$- and the $\mathcal{R}^{\mathrm{sr}}$-synthesizability problem for $\mathcal{G}$

Let $\mathcal{S}$ be a set of 1-fold, unfragmented, building n-rules and G, H be n-multigraphs.

Proposition 3.12 *Assume that* $\mathrm{dom}(H) \subseteq \mathrm{dom}(G)$*. H is a closed $\mathcal{S}$-product of G iff* $\mathrm{dom}(H)$ *is closed in G and H is $\mathcal{S}$-synthesizable from* $G|\mathrm{dom}(H)$*.*

Proof. $\Leftarrow$ follows from Proposition 3.4. $\Rightarrow$. Let $G_0, \ldots, G_l$ be an $\mathcal{S}$-synthesis from G and H a closed substructure of G_l. $\mathrm{dom}(H)$ is the union of the components of G_l contained in $\mathrm{dom}(H)$. With Corollary 3.6 $\mathrm{dom}(H)$ is closed in every G_i $(0 \leq i \leq l)$, hence in G_0. With Corollary 3.2 $G_0|\mathrm{dom}(H), \ldots, G_l|\mathrm{dom}(H)$ is an $\mathcal{S}$-synthesis. $\diamondsuit$

Corollary 3.8 *H is a closed $\mathcal{S}$-product of a combination of G iff it is $\mathcal{S}$-synthesizable from a combination of restrictions of G to one of its components.*

Proof. Immediate from Proposition 3.12, given that G and any combination of G have, up to isomorphism, the same restrictions to a component. $\diamondsuit$

Corollary 3.9 *The closed $\mathcal{R}^{\mathrm{ub}}$-synthesizability problem for $\mathcal{G}$ is solvable.*

Proof. Immediate from Corollary 3.8. $\diamondsuit$

We turn now our attention to separating n-rules.

Let $\mathcal{S}$ be a set of separating n-rules and G a finite n-multigraph. We will obtain, up to isomorphism, all restrictions of an n-multigraph $\mathcal{S}$-synthesizable from a combination of G to one of its components. For simplicity we assume that all n-rules in $\mathcal{S}$ are unfragmented. It is not difficult to adapt the definition of $\mathcal{C}_i$ to the case of finite, separating n-rules (in this case a P-shift of a k-combination, for a k-fold $P \in \mathcal{S}$, which is used in the definition, is not necessarily correct anymore, if P is fragmented). Define $\mathcal{C}_0$ to be the set of the restrictions of G to one of its components and for all $i \in \mathbb{N}$

$$\begin{aligned}\mathcal{C}_{i+1} \quad = \quad \mathcal{C}_i \cup \{K \mid \quad & K \text{ is the isomorphism type of a restriction to a component} \\ & \text{of a } P\text{-shift of a } k\text{-combination of } \mathcal{C}_i \text{ for a } k\text{-fold } P \in \mathcal{S}\}.\end{aligned}$$

Proposition 3.13 *There is $i \in \mathbb{N}$ for which $\mathcal{C}_{i+1} = \mathcal{C}_i$ and $\mathcal{C}_i$ is the set of all isomorphism types of the restrictions to a component of an n-multigraph $\mathcal{S}$-synthesizable from a combination of G.*

Proof. We sketch the proof and leave the details to the reader. If (K, a) is a k-fold, separating n-rule, then $\mathrm{cl}_{\mathrm{sh}(K,a_0,\ldots,a_{4i-1})}(a_{4i}) = \mathrm{cl}_{\mathrm{sh}(K,a_0,\ldots,a_{4i-1})}(\{a_{4i}, a_{4i+1}, a_{4i+2}, a_{4i+3}\})$ $(0 \leq i < k)$. Thus, if $P \in \mathcal{S}$ is k-fold, H an n-multigraph and $\bar{H}$ a P-shift of H, then every component of $\bar{H}$ is contained in a component of H and there are components $A_0, \ldots, A_{k-1}$ of H such that $\bar{H}$ is the sum of a P-shift of $H|(A_0 \cup \ldots \cup A_{k-1})$ and $H|\mathrm{dom}(H) \setminus (A_0 \cup \ldots \cup A_{k-1})$. $\diamondsuit$

Proposition 3.14 *The $\mathcal{R}^{\mathrm{sr}}$-synthesizability problem for $\mathcal{G}$ is solvable.*

Proof. The procedure computes i and $\mathcal{C}_i$ of Proposition 3.13. For any n-multigraph H, if H is a substructure of a combination of $\mathcal{C}_i$, H is an $\mathcal{S}$-product of a combination of G; otherwise, it is not. $\diamondsuit$

3.4 Solvability of the basic addition problem

In this section we prove the solvability of the basic addition problem. The solvability of this problem is not obvious. It is not inherent to the nature of additions, as one may think. To the contrary, if we just would allow 12-element, 2-fold additions, instead of only basic additions, which are 4-element, 1-fold additions, the problem would turn undecidable, as we will see in Chapter 5. The proof, if carried out in a formally correct way, requires, but at the same time offers a good opportunity to practice, some elementary set theoretic calculation.

For the whole Section 3.4 let $n \in \mathbb{N}$, d: $\{0, \ldots, n\} \to \mathbb{N}$ and $D = \max\{d(0), \ldots, d(n)\}$.

Let G, H be n-multigraphs with degree requirement d, $A \subseteq \mathrm{dom}(G)$, f an A-homomorphism from G to H, $P := (K, z)$ a basic n-addition and $H' = P\text{-sh}(H, (a, b, c, d))$ $(a, b, c, d \in \mathrm{dom}(H))$. We abbreviate $B = f(A)$, $F(u) = \{v \in \mathrm{nb}_{_G}(A) \mid f(v) = u\}$ $(u \in \mathrm{nb}_{_H}(B))$.

Lemma 3.1 *Suppose that $a \in B$ and $\{c, d\} \cap B \neq \emptyset$. Then $f|\mathrm{nb}_{_{G'}}(A)$ is an A-homomorphism from a P-shift G' of G to H'.*

Proof. We assume $H' \neq H$, otherwise the claim trivially holds for $G' = G$. There are $a' \in A$, $b' \in \mathrm{nb}_{_G}(a')$, c', d' with $\{c', d'\} \cap A \neq \emptyset$, $d' \in \mathrm{nb}_{_G}(c')$ such that $f(a'), f(b'), f(c'), f(d') = a, b, c, d$. It is easy to conclude that there is an embedding from (K, z) into $(G, (a', b', c', d'))$. Take $G' = \mathrm{sh}(G, (a', b', c', d'))$. It is rather immediate that $f|A$ is a partial isomorphism from G' to H'. We prove that

$$\mathrm{nb}_{_{G'}}(u) \subseteq \mathrm{nb}_{_G}(u) \text{ and } f(\mathrm{nb}_{_{G'}}(u)) = \mathrm{nb}_{_{H'}}(f(u)) \text{ for all } u \in A. \tag{1}$$

(Regarding $\mathrm{nb}_{_{G'}}(A) \subseteq \mathrm{nb}_{_G}(A)$, as an exercise, using Proposition 3.1 and by distinguishing between $d' \in A$ and $c' \in A$, it can actually be formally proven that $\mathrm{nb}_{_G}(A) = \mathrm{nb}_{_{G'}}(A) \cup \{b', c'\}$).

To begin we distinguish between $u \in A \setminus \{a', b', c', d'\}$ and $u \in A \cap \{a', b', c', d'\}$. Assume $u \in A \setminus \{a', b', c', d'\}$.

Lemma 3.2 $f(u) \notin \{a, b, c, d\}$.

Proof. Towards a contradiction suppose $f(u) = c$. Then $f(u) = f(c')$. Since $u \neq c'$ and $f|A$ is injective, $c' \notin A$, whence $d' \in A$, which yields $c' \in \mathrm{nb}_{_G}(A) \setminus A$. By Proposition 2.32

for all $\mathcal{S}$-synthesizable H from a combination of G and all $B \subseteq \mathrm{dom}(H)$ with $|B| = m$ there are $j \leq k$, an $\mathcal{S}$-synthesizable K from a j-combination of G and $A \subseteq \mathrm{dom}(K)$ with (K, A) neighbour equivalent to (H, B). Now, if (K, A) is neighbour equivalent to (H, B) then, obviously, there is an A-homomorphism from K to H with $f(A) = B$. This short discussion leads to the following theorem:

Theorem 3.2 *The basic addition problem is solvable.*

Proof. We outline a procedure that for a set $\mathcal{S}$ of basic n-additions (that indeed we can assume to be finite) and finite n-multigraphs G, H, where G has degree requirement d, decides whether H is an $\mathcal{S}$-product of a combination of G. Let $m = \max\{|\mathrm{dom}(H)|, 4\}$, $D = \max\{d(0), \ldots, d(n)\}$ and $M = (\frac{m \cdot D}{2})^2$. The procedure finds $k \in \mathbb{N}$, $k \geq m$ with the property that for all $k < i \leq (M+1)k$ every neighbour equivalence type of a (K, A), where K is $\mathcal{S}$-synthesizable from a i-combination of G and $|A| = m$, is the type of a (J, B) where, for some $j \leq k$, J is $\mathcal{S}$-synthesizable from an j-combination of G. This k exists from the short discussion leading to Theorem 3.2. Then it checks whether H is an $\mathcal{S}$-product of an i-combination of G for $i \leq k$. Since all $i \leq (M+1)k$ reduce to k, by Theorem 3.1, all $i \in \mathbb{N}$ reduce to k. This proves that, if H is an $\mathcal{S}$-product of a combination of G, the check must be positive. $\diamondsuit$

4 The Shift Theorem

The Shift Theorem, that is proven in this chapter, fully characterizes the shift operation. A consequence of the Shift Theorem is the solvability of the most immediate, particular case of the synthesizability problem.

In order to prove the theorems in this section we generalize the definition of n-multigraph and shift.

A *multigraph* (respectively a *natural multigraph*) on the set A is a symmetric function $G: A^2 \to \mathbb{Z} = \{\ldots -2, -1, 0, 1, 2\ldots\}$, i. e. a function $G: A^2 \to \mathbb{Z}$ with $G(a, b) = G(b, a)$ for all $a, b \in A$ (respectively a symmetric function $G: A^2 \to \mathbb{N}$). An element of A is called a *point* of the multigraph G on A. A (*natural*) *multigraph* is a (natural) multigraph on some set.

Let G be a multigraph on A. G is said to be *finite* iff A is finite. If G is finite, the number

$$\deg_G(a) = \sum_{b \in A \setminus \{a\}} G(a, b)$$

is called the *degree* of a in G. The finite multigraphs G, H on a common set A are called *similar* iff the value and the degree of any point are the same in both G and H, i.e. iff

$$G(a, a) = H(a, a) \text{ and } \deg_G(a) = \deg_H(a)$$

for all $a \in A$.

The *shift* of the multigraph G on A at the distinct elements $a_0, a_1, a_2, a_3 \in A$, $\mathrm{sh}(G, a_0, a_1, a_2, a_3)$, is the multigraph H on A that satisfies:

$a \notin \{a_0, \ldots, a_m\}$ with $G(a_m, a) > 0$. For $0 \leq i \leq m-2$ the values of G are

$$a \overset{>0}{\text{---}} a_m \overset{<0}{\text{---}} a_{m-1} \overset{>0}{\text{---}} a_i,$$

which with statement (1) implies $G(a, a_i) > 0$. Moreover

$$a \overset{>0}{\text{---}} a_m \overset{<0}{\text{---}} a_{m-2} \overset{>0}{\text{---}} a_{m-1},$$

which again with (1) implies $G(a, a_{m-1}) > 0$. $\diamondsuit$

By Lemma 4.2 there is a circular sequence b_0, b_1, b_2 in G. Assume $G(b_0, b_1) > 0$ (otherwise use $-G$). Obviously b_2, b_1, b_0 switches and with Lemma 4.3 we conclude that G is infinite, which is a contradiction. Hence Lemma 4.1 holds. $\diamondsuit$

Let $n \in \mathbb{N}$. A natural multigraph G on A is called *bound* iff $G(a,b) \leq n$ for all $a \neq b$ in A.

Theorem 4.2 (Shift Theorem) *Let G, H be finite, similar, natural, bound multigraphs. Then there is a sequence $G_0, \ldots, G_l$ of natural, bound multigraphs, where $G_0 = G$, $G_l = H$ and G_{i+1} is a shift of G_i for all $0 \leq i < l$.*

Proof. Define δ as in the proof of Theorem 4.1:

$$\delta(G, H) = \sum_{\{a,b\} \in [A]^2} |G(a,b) - H(a,b)|.$$

($[A]^2$ is the set of 2-element subsets of A.) The proof is by induction on the value of $\delta(G, H)$. If $\delta(G, H) = 0$, then $G = H$. Assume that the theorem holds, if $\delta(G, H) \leq j$ and let $\delta(G, H) = j + 1$.

5 Undecidability of the synthesizability problem

In this chapter two undecidable variations of the word problem for Semi-Thue systems are reduced each one to a case of the synthesizability problem, which implies the unsolvability of the two latter cases.

As in Chapter 2, $\mathrm{S}_n = \{R_1, \dots, R_n\}$. S_n is intended as an alphabet. We define $\tilde{\mathrm{S}}_n = \{R_3, \dots, R_n\} = \mathrm{S}_n \setminus \{R_1, R_2\}$.

Let Σ be an alphabet and w, v be in the set Σ^* of all words over Σ. The *reversal* $\tilde{w}^\Sigma$ of w (*with respect* to Σ) is the word w written in the opposite direction (from right to left), i. e., if $w_0, \dots, w_{i-1} \in \Sigma$ and $w = w_0 \dots w_{i-1}$, $\tilde{w}^\Sigma = w_{i-1}w_{i-2} \dots w_0$. v is w-*oriented* (*with respect* to Σ) iff $\tilde{w}^\Sigma$ is not a subword of v. If A is a set of words over Σ, v is A-*oriented* (*with respect* to Σ) iff it is w-oriented for every $w \in A$.

A *semi-Thue system* (over Σ) [1] is a pair (Σ, ρ), where Σ is an alphabet and ρ is a finite subset of $(\Sigma^*)^2$. Let $\mathcal{T} = (\Sigma, \rho)$ be a semi-Thue system. If $w, v \in \Sigma^*$, we call w a $\mathcal{T}$-*rewriting* of v iff there are $s, t, y, z \in \Sigma^*$ such that $v = syt$, $w = szt$ and $(y, z) \in \rho$. The reflexive transitive closure over Σ^* of the $\mathcal{T}$-rewriting relation is called the $\mathcal{T}$-*reduction* relation. Said differently, w is a (l-*step*) $\mathcal{T}$-*reduction* of v iff there is an $l+1$-sequence u to Σ^* with $u_0 = v$, $u_l = w$ and u_{i+1} is a $\mathcal{T}$-rewriting of u_i $(0 \le i < l)$. Denote by A the set $\{y \,|\, \text{there is } z \text{ with } (y, z) \in \rho\}$. $v \in \Sigma^*$ is called $\mathcal{T}$-*oriented* iff every $\mathcal{T}$-reduction of v is A-oriented. The *word* problem for $\mathcal{T}$ is the question:

Given $v, w \in \Sigma^*$ is w a $\mathcal{T}$-reduction of v?

Theorem 5.1 *There are semi-Thue systems $\mathcal{T} = (\Sigma, \rho)$, $\mathcal{I} = (\Sigma, \sigma)$ with $|\Sigma| = 12$ and an $\mathcal{I}$-oriented $w = w_0 w_1 w_2 w_0$ $(w_0, w_1, w_2 \in \Sigma)$ such that $|y|_\Sigma, |z|_\Sigma \leq 4$ and $|y|_\Sigma \geq 2$ for all $(y, z) \in \rho \cup \sigma$, no procedure decides for all $\mathcal{T}$-oriented $v \in \Sigma^*$ whether the empty word $\emptyset$ is a $\mathcal{T}$-reduction of v and no procedure decides for all $v \in \Sigma^*$ whether v is a $\mathcal{I}$-reduction of w.*

Proof. We first prove the existence of $\mathcal{T}$. We follow the idea of Post to reduce the halting problem for a Turing machine to the word problem for a semi-Thue system [3], [2]. The theorem then follows by considering that the halting problem for a universal Turing machine is not decidable (i. e. the set of words on which the machine halts is not recursive) and that there is a universal Turing machine with 4 states and a 6-element tape alphabet [7], [8]. At this point I would like to remark that the undecidability of the word problem for a semi-Thue system has been proven also by Markov [9]. The undecidability of the halting problem for a universal Turing machine follows from the existence of a Turing machine with undecidable halting problem, which, in turn, follows from the fact that every recursively enumerable set is the set accepted by a Turing machine and that there are recursively enumerable sets that are not recursive (like the set of logical identities or the set of finitely satisfiable sentences). The undecidability of the halting problem for a universal Turing machine follows also from Turing's Theorem that the set of words Mz, where M is a Turing machine that accepts z, is not recursive [6], [5].

What is left now is to prove the reduction mentioned at the beginning of the proof. To achieve this goal we first associate to a Turing machine M a semi-Thue system $\mathcal{T} = (\Sigma, \rho)$ in such a way that, for an effective (and simple) transformation of an input word of the Turing machine into a $\mathcal{T}$-oriented word over Σ, M halts on an input word iff w is a $\mathcal{T}$-reduction of its transformation. The association is a slight modification of Post's association and is defined in the following way. Let M have tape alphabet Γ with the blank 0, set of states S with s_0 the start state, s_1 the halt state and next move function $\delta : X \subseteq \Gamma \times S \to \Gamma \times S \times \{L, R\}$.

$$\begin{aligned}
\text{We set}\quad \Sigma &= \Gamma \cup S \cup \{>, |\}\ (>, | \notin \Gamma \cup S) \text{ and}\\
\rho &= \{(q > a, bq' >) \,|\, (a,q) \in X \text{ and } \delta(a,q) = (b, q', R)\} \cup\\
&\quad\ \{(cq > a, q' > cb) \,|\, c \in \Gamma, (a,q) \in X \text{ and } \delta(a,q) = (b, q', L)\} \cup\\
&\quad\ \{(|q >, |0q >) \,|\, q \in S\} \cup \{(q > |, q > 0|) \,|\, q \in S\} \cup\\
&\quad\ \{(s_1 > a, s_1 >) \,|\, a \in \Gamma\} \cup \{(as_1 >, s_1 >) \,|\, a \in \Gamma\} \cup \{(|s_1 > |, \emptyset)\}.
\end{aligned}$$

The pairs in the third line are added to allow the tape to be endless on both side, the pairs in the last line to make the empty word the unique accepting word. It is left to the reader to ascertain that $\emptyset$ is a $\mathcal{T}$-reduction of the $\mathcal{T}$-oriented $|s_0 > z|$ iff M halts on the input word z of M.

The existence of $\mathcal{I}$ is proven by taking $\sigma = \{(y, z) \,|\, (z, y) \in \rho \text{ and } y \neq \emptyset\}$ and $w = |s_1 > |$. $\diamondsuit$

A *word n-multigraph* ($n \neq 0$) is a 1-bound n-multigraph G with $\mathrm{dom}(G) = \{0, \ldots, k\}$

($k \in \mathbb{N}$) such that for all $0 \leq i < j \leq k$

$$\text{if } j = i + 1,\ R_1^G(i, j);$$

$$\text{if } j \neq i + 1,\ \mathrm{val}_G(i, j) = 0.$$

If G is a k-element word n-multigraph and $0 \leq i \leq n$, the *i-termination* of G is the $(k + 1)$-element word n-multigraph $H \supseteq G$ with $\mathrm{val}_H(k, k) = i$.

5.1 Word representations

For this whole section let $n \in \mathbb{N}, n \geq 2$.

Let $v_0, \ldots, v_{i-1} \in \mathrm{S}_n$, $v = v_0 \ldots v_{i-1}$. For $i > 0$ the *natural n-representation* of v, $\mathrm{nrp}_n(v)$, is the i-element word n-multigraph G satisfying $v_j^G(j, j)$ $(0 \leq j < i)$. The *second* (respectively *third*) *n-representation* of v, $\mathrm{srp}_n(v)$ (respectively $\mathrm{trp}_n(v)$), is the 0-termination of the $i + 1$-element word n-multigraph G satisfying

$$v_j^G(j + 1, j + 1)\ (0 \leq j < i) \text{ and}$$

$$R_1^G(0, 0) \text{ (respectively } R_2^G(0, 0)).$$

Obviously, if $w \in \tilde{\mathrm{S}}_n^*$, $|w|_{\tilde{\mathrm{S}}_n} \geq 1$ and $\mathrm{nrp}_n(w)$ is embedded into $\mathrm{nrp}_n(v)$ ($|v|_{\mathrm{S}_n} \geq 1$), $\mathrm{srp}_n(v)$ or $\mathrm{trp}_n(v)$, then w or $\tilde{w}$ is a subword of v. Consequently, if v is w-oriented, then $\mathrm{nrp}_n(w)$ is embedded into $\mathrm{nrp}_n(v)$ iff w is a subword of v.

Proposition 5.1 *$\mathrm{srp}_n(v)$ and $\mathrm{trp}_n(v)$ are in $\mathcal{G}_{d_n}$ for all $v \in \tilde{\mathrm{S}}_n^*$.*

Proof. Left to the reader. The function d_n was introduced in section 3.2. $\diamondsuit$

A *second* (*third*) *n-representation* is an n-multigraph isomorphic to $\mathrm{srp}_n(v)$ ($\mathrm{trp}_n(v)$) for some $v \in \tilde{\mathrm{S}}_n^*$. An *n-representation* is a combination of the class of all second or third n-representations.

If $G = \mathrm{srp}_n(v)$ (or $G = \mathrm{trp}_n(v)$) and $|G| = i + 2$, then $\mathrm{nb}_G^j(0) = \{0, \ldots, j\}$ $(0 \leq j \leq i+1)$, whence $\mathrm{nb}_G^{i+1}(0) = \mathrm{dom}(G)$, and $\mathrm{nb}_G^{i+2}(0) = \mathrm{nb}_G^{i+1}(0)$. Thus all second or third n-representations are connected. It is left to the reader to prove that no proper extension of a second or third n-representation is a second or third n-representation. Therefore Proposition 2.25, Proposition 2.26 and Proposition 2.27 are correct for the class $\mathcal{C}$ of all second or third n-representations and for the class $\mathcal{D}$ of all n-representations. In particular the following statement is correct.

Proposition 5.2 *A substructure of an n-representation H is a closed substructure of H iff it is an n-representation.* ◊

Let $v_0, \ldots, v_{i-1} \in \mathrm{S}_n$, $v = v_0 \ldots v_{i-1}$, $w \in \mathrm{S}_n^*$ be of length j. The *addition n-representation* $\mathrm{arp}_n^{k,l}(v, w)$ of (v, w) with $1 \leq k \leq n$, $0 \leq l \leq n$ is the 2-fold, 1-bound n-addition

$$(K \oplus U, a),$$

where K is the l-termination of $\mathrm{ngr}_n(R_k v)$, the mapping assigning $i+2, \ldots, i+j+3$ to

$G_1, h(a_0), \ldots, h(a_7))$. $\diamondsuit$

On the other hand, the following lemma holds:

Lemma 5.2 *Assume that $v \in \tilde{\mathrm{S}}_n^*$ is y-oriented, $\mathrm{srp}_n(w)$ is embedded into an $\mathrm{arp}_n(y,z)$-shift H of $G := (\mathrm{srp}_n(v) \oplus G_0)$, where G_0 is a third n-representation with domain disjoint from $\mathrm{dom}(\mathrm{srp}_n(v)) = \{0, \ldots, |v|_{\tilde{\mathrm{S}}_n} + 1\}$. Then $w = v$ or w is a $(\mathrm{S}_n, \{(y,z)\})$-rewriting of v.*

Proof. If $H = G$, $\mathrm{srp}_n(w) \cong \mathrm{srp}_n(v)$, because $\mathrm{srp}_n(w)$ is embedded into G. This implies $w = v$. We consider the case $H \neq G$. Then there is an n-addition $(K, a) \in \mathrm{arp}_n(y,z)$ and an embedding f from K into G with $H = \mathrm{sh}(G, f(a_0), \ldots, f(a_7))$. Indeed, $\{f(i{+}2), \ldots, f(i{+}j{+}3)\} = \mathrm{dom}(G_0)$. Therefore $0 \leq f(k) < |v|_{\tilde{\mathrm{S}}_n}{+}2$ for all $0 \leq k \leq i{+}1$ and, since v is y-oriented, $f(k+1) = f(k) + 1$ for all $0 \leq k \leq i$. By looking at the definition of an addition n-representation of (y,z) we obtain that $H = H_0 \oplus H_1$, where H_0, H_1 have disjoint domains, $H_0 \cong \mathrm{srp}_n(w')$ for a $\{(y,z)\}$-rewriting w' of v and H_1 is a third n-representation. $\mathrm{srp}_n(w) \cong H_0$, because $\mathrm{srp}_n(w)$ is embedded into H. This implies $w = w'$ and consequently w is a $\{(y,z)\}$-rewriting of v. $\diamondsuit$

5.2 Reduction of the word problem to the synthesizability problem

Let $n \in \mathbb{N}, n \geq 2$, $\Sigma \subseteq \mathrm{S}_n$, $v, w \in \Sigma^*$ and $\mathcal{T} = (\Sigma, \rho)$ be a semi-Thue system. The $l+1$-sequence $\mathcal{G}$ is *built on* $(n, \mathcal{T}, v, w)$ iff

(i) $\mathcal{G}_0 = \{\mathrm{srp}_n(v)\} \cup \{\mathrm{trp}_n(z) \mid (y,z) \in \rho \text{ for some } y \in \Sigma^*\}$.

(ii) $\mathcal{G}_{i+1} = \mathcal{G}_i \cup \{H\}$, where H is an $\mathrm{arp}_n(\mathcal{T})$-shift of a finite combination of $\mathcal{G}_i$ $(0 \leq i < l)$.

(iii) $\mathrm{srp}_n(w)$ is embedded into some $G \in \mathcal{G}_l$.

Theorem 5.2 (a) *Assume that w is a k-step $\mathcal{T}$-reduction of v. Then there is a $k+1$-sequence built on $(n, \mathcal{T}, v, w)$.*

(b) *Assume that $\Sigma = \tilde{\mathrm{S}}_n$ and v is $\mathcal{T}$-oriented. Then w is a $\leq k$-step $\mathcal{T}$-reduction of v iff there is an $l+1$-sequence $\mathcal{G}$ built on $(n, \mathcal{T}, v, w)$ $(l \leq k)$.*

Proof. (a) There is a $k+1$-sequence u to Σ^* with $u_0 = v$, $u_k = w$ and u_{i+1} a $\mathcal{T}$-rewriting of u_i $(0 \leq i < k)$. We want to show that there is a $k+1$-sequence built on $(n, \mathcal{T}, v, w)$. The proof is by induction on k, the case $k = 0$ being obvious. Assume the case $k = l$ holds for all $w \in \Sigma^*$. Let $k = l + 1$. $w = u_k$ is a $(\mathrm{S}_n, \{(y, z)\})$-rewriting of $u_l \in \Sigma^*$ for some $(y, z) \in \rho$. By induction hypothesis there is an $l+1$-sequence $\mathcal{G}$ built on $(n, \mathcal{T}, v, u_l)$. $\mathrm{srp}_n(u_l)$ is embedded into some $G_0 \in \mathcal{G}_l$. Let $G_1 \cong \mathrm{trp}_n(z)$ have domain disjoint from $\mathrm{dom}(G_0)$. $G_0 \oplus G_1$ is a finite combination of $\mathcal{G}_l$ and, by Lemma 5.1, $\mathrm{srp}_n(w)$ is embedded into an $\mathrm{arp}_n(y, z)$-shift H of $G_0 \oplus G_1$. This means that the $l+2$-sequence $\mathcal{G}_0, \ldots, \mathcal{G}_l, \mathcal{G}_l \cup \{H\}$ is built on $(n, \mathcal{T}, v, w)$.

(b) $\Rightarrow$ is immediate from (a). $\Leftarrow$. Assume there is an $l+1$- sequence $\mathcal{G}$ built on $(n, \mathcal{T}, v, w)$. We claim that w is a $\leq l$-step $\mathcal{T}$-reduction of v. This goes again by induction on l and is easy, if $l = 0$. Assume the claim is true for $l = k$. Set $l = k + 1$. Every no procedure decides for all $\mathcal{T}_0$-oriented $v \in \tilde{\mathrm{S}}_{14}^*$ whether the empty word $\emptyset$ is a $\mathcal{T}_0$-reduction of v and

no procedure decides for all $v \in \tilde{\mathrm{S}}_{14}^*$ whether v is a $\mathcal{I}_0$-reduction of t_0.

Recall that $d_{14}\colon \{0,\dots,14\} \to \{1,2\}$ maps $0,1,2$ to 1 and $3,\dots,14$ to 2. $\mathrm{srp}_{14}(\emptyset) \in \mathcal{G}_{d_{14}} \cap \mathcal{G}^1 \cap \mathcal{G}^{\mathrm{conn}}$ has a 2-element domain. Using Proposition 5.3, $\mathrm{arp}_{14}(\mathcal{T}_0) \neq \emptyset$ and $\mathrm{arp}_{14}(\mathcal{I}_0) \neq \emptyset$ are finite sets of 2-fold, 1-bound 14-additions (K,u) with $\max\{|\mathrm{dom}(K)| - |\{u_0,\dots,u_7\}|\} \leq 4$.

Let $\mathcal{H}$ be a set of structures with pairwise disjoint domains whose isomorphism types are precisely the types of the structures in $\{\mathrm{srp}_{14}(t_0)\} \cup \{\mathrm{trp}_{14}(z) \mid (y,z) \in \rho_0 \text{ for some } y \in \tilde{\mathrm{S}}_{14}^*\}$. $\mathcal{H}$ can be chosen to be a finite set of at most 6-element structures in $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1 \cap \mathcal{G}^{\mathrm{conn}}$. Set $H_0 = \sum \mathcal{H}$. $H_0 \in \mathcal{G}_{d_{14}} \cap \mathcal{G}^1$.

Corollary 5.3 *The* $\mathrm{arp}_{14}(\mathcal{T}_0)$*-synthesizability problem for* $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1, \mathrm{srp}_{14}(\emptyset)$ *and the* $\mathrm{arp}_{14}(\mathcal{I}_0)$*-synthesizability problem for* H_0, $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1 \cap \mathcal{G}^{\mathrm{conn}}$ *are unsolvable.*

Proof. We use the rewriting of the synthesizability problem stated at the beginning of Section 3.2. $\mathrm{srp}_{14}(v)$ and $\mathrm{trp}_{14}(v)$ are in $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1$ for all $v \in \tilde{\mathrm{S}}_{14}^*$. Therefore, if the procedure P solves the $\mathrm{arp}_{14}(\mathcal{T}_0)$-synthesizability problem for $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1, \mathrm{srp}_{14}(\emptyset)$, we can obtain a procedure P_0 that decides for $v \in \tilde{\mathrm{S}}_{14}^*$ in the same way P decides given $14, \mathrm{arp}_{14}(\mathcal{T}_0), \{\mathrm{srp}_{14}(v)\} \cup \{\mathrm{trp}_{14}(z) \mid (y,z) \in \rho_0 \text{ for some } y \in \tilde{\mathrm{S}}_{14}^*\}, \mathrm{srp}_{14}(\emptyset)$. With Corollary 5.2 for any $\mathcal{T}_0$-oriented $v \in \tilde{\mathrm{S}}_{14}^*$ the procedure P_0 decides whether $\emptyset$ is a $\mathcal{T}_0$-reduction of v, which creates a contradiction.

If the procedure P solves the $\mathrm{arp}_{14}(\mathcal{I}_0)$-synthesizability problem for $H_0, \mathcal{G}_{d_{14}} \cap \mathcal{G}^1 \cap \mathcal{G}^{\mathrm{conn}}$, we can obtain a procedure P_0 that decides for $v \in \tilde{\mathrm{S}}^*_{14}$ in the same way P decides given $14, \mathrm{arp}_{14}(\mathcal{I}_0), H_0, \mathrm{srp}_{14}(v)$. Since t_0 is $\mathcal{I}_0$-oriented, with Corollary 5.2, P_0 decides whether v is a $\mathcal{I}_0$-reduction of t_0, which creates again a contradiction. $\diamondsuit$

Corollary 5.4 *The (2-fold) addition (and thus the synthesizability) problem is unsolvable.* $\diamondsuit$

It is worthwhile pointing out at this point that the question whether the 1-fold synthesizability (or even addition) problem is solvable or not remains open in this work.

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6 A condition for m-equivalence between structures over a set of relation symbols or constants

Mathematicians have found several conditions equivalent to or stronger than the m-equivalence between structures ($m \in \mathbb{N}$), i. e. the property of satisfying the same sentences of quantifier rank m. If the underlying set of symbols is a finite set of relation symbols or constants, Fraïssé proved that m-equivalence is equivalent to the existence of an m-back-and-forth system between the structures [5, 1, 4]. Ehrenfeucht gave a characterization based on the existence of a winning strategy for the second player in the game that carries his name [2, 1, 4]. Still under the assumption that the underlying set of symbols is a finite set of relation symbols or constants, all m-equivalence classes are axiomatized by a sentence, called *m-Hintikka sentence* [1, 4], or, more specifically, the *m-Hintikka sentence* of the class. It follows that two structures are m-equivalent iff there is an m-Hintikka sentence that they both satisfy. Finally Hanf [3, 1], using Ehrenfeucht's game, found a stronger condition based on the number of the isomorphism types of the 2^m-neighbourhoods [6] (3^m-neighbourhoods in [1]) in a graph constructed from the structures.

Equivalence relations, like the r, m-equivalence, that are naturally derived from the m-equivalence, are fundamental for our investigation of synthesizability. Therefore it appeared appropriate to investigate them as well. This is what we do in this chapter. We provide another sufficient condition for m-equivalence. This condition allows us to significantly strengthen Hanf's Theorem. Using, as an example, the class of structures that are a k-path for some $k \in \mathbb{N}$ and the related class $\mathcal{U}$, which is the class of structures that are an alternate k-path for some even $k \in \mathbb{N}$ or the class of structures that are an alternate k-path for some odd $k \in \mathbb{N}$, we obtain, through this strenghtening, depending on arbitrary $r, m \in \mathbb{N}$, in Theorem 6.2, the smallest k such that for all $j \geq k$ all j-paths are pairwise r, m-equivalent, in Theorem 6.3, the smallest k such that for all $j \geq k$ all j-paths are pairwise $2, r, m$-equivalent, in Proposition 6.19, a number at most $r + 1$ (if $r \neq 0$) above the smallest k such that for all $j \geq k$ all alternate j-paths in $\mathcal{U}$ are pairwise r, m-equivalent and finally, in Proposition 6.21, for even r, a number at most $\frac{r}{2} + 1$ (if $r \neq 0$) above the smallest k such that for all $j \geq k$ all alternate j-paths in $\mathcal{U}$ are pairwise $2, r, m$-equivalent.

These achievements will lead in their turn to practicable conclusions regarding the derivability in a fixed number of steps from combinations of sets of structures belonging to or constructed from the structures in the classes used as an example. These conclusions are presented in Section 7.3.

Until the end of Section 6.1 let L be a set of relation symbols, C a set of constants and $e \notin \mathrm{C}$ a constant.

Let U be a structure over $\mathrm{L} \cup \mathrm{C}$, $u \in \mathrm{dom}(U)$, $A \subseteq \mathrm{dom}(U)$, $\mathrm{C}_0 \subseteq \mathrm{C}$ and $k \in \mathbb{N}$. We will use the following definitions and simplifications of notation:

$\mathrm{C}_0^U = \{c^U \mid c \in \mathrm{C}_0\}$,

$U|A = (U \restriction \mathrm{L})|A \ (A \neq \emptyset)$,

$\mathrm{gf}(U) = \mathrm{gf}(U \restriction \mathrm{L})$,

$\mathrm{nb}^k_U(A) = \mathrm{nb}^k_{\mathrm{gf}(U)}(A)$,

$\mathrm{nb}^k_U(u) = \mathrm{nb}^k_U(\{u\})$,

$U^k(A) = (U|(\mathrm{nb}^k_U(A) \cup \mathrm{C}^U), (c^U)_{c \in \mathrm{C}})$,

$U^k(u) = U^k(\{u\})$.

The *k-neighbourhood type* of u in U is the isomorphism type of $(U^k(u), (e{:}\, u))$.

Indeed, the smallest k for which $a \in \mathrm{nb}^k_U(b)$, if there is such a k, ∞, otherwise, satisfies the conditions of a distance between a and b (depending on U). We will not work with the distance, because in spite of its intuitive value, it does not effectively simplify the proofs.

Proposition 6.1 *For all $a, b, c \in \mathrm{dom}(U)$ if $a \in \mathrm{nb}^k_U(b)$ and $a \in \mathrm{nb}^j_U(c)$, then $c \in \mathrm{nb}^{k+j}_U(b)$.*

Proof. By induction on k. ♢

Proposition 6.2 *Let $j \in \mathbb{N}$ and $j \leq k$. $\mathrm{nb}^j_U(u) = \mathrm{nb}^j_{U|\mathrm{nb}^k_U(u)}(u)$.*

Proof. This proposition is a particular case ($A = \{u\}$) of Proposition 2.21 (d). ♢

6.1 m-overlaps

Let U, V be structures over $\mathrm{L} \cup \mathrm{C}$ and $m \in \mathbb{N}$. We define an *m-overlap* from U to V as a triple

$$((a_1, \ldots, a_i), (b_1, \ldots, b_i), (p_1, \ldots, p_i))$$

$\mathrm{nb}_V^{2^{m-i-1}}(\{b_1, \ldots, b_i\})$ there is $a \in \mathrm{dom}(U)$ such that

$$((a_1, \ldots, a_i, a), (b_1, \ldots, b_i, b), (p_1, \ldots, p_i, p)) \in \mathcal{O}$$

for some p.

Theorem 6.1 *If there is an m-neighbourhood system from U to V, which is closed under m-extensions from U to V, then $U \equiv_m V$.*

Proof. Assume that $\mathcal{O}$ is an m-neighbourhood system from U to V, which is closed under m-extensions from U to V. Let $0 \leq i < m$ and suppose that in an Ehrenfeucht-Fraïssé m-game U, V after exactly i moves the play $(a, b) = ((a_1, \ldots, a_i), (b_1, \ldots, b_i))$ has been made with $(a, b, p) \in \mathcal{O}$ for some p. We show that for every $u \in \mathrm{dom}(U)$ there is $v \in \mathrm{dom}(V)$ and vice versa such that $((a, u), (b, v), (p, q)) \in \mathcal{O}$ for some q. By Proposition 6.4 (c) this gives Duplicator a winning strategy in the game. Ehrenfeucht's Theorem yields subsequently the claim.

If $u \in \mathrm{nb}_U^{2^{m-i-1}}(a_j)$ for some $1 \leq j \leq i$, then set $v = p_j(u)$. The m-extension $((a, u), (b, v), (p, p_j|\mathrm{dom}(U^{2^{m-i-1}-1}(u))))$ of (a, b, p) is therefore in $\mathcal{O}$. If $v \in \mathrm{nb}_V^{2^{m-i-1}}(b_j)$ for some $1 \leq j \leq i$, then $v = p_j(u)$ for some $u \in \mathrm{dom}(U^{2^{m-j}-1}(a_j))$. By Proposition 6.3 $u \in \mathrm{nb}_U^{2^{m-i-1}}(a_j)$. Again $((a, u), (b, v), (p, p_j|\mathrm{dom}(U^{2^{m-i-1}-1}(u))))$ is an m-extension of (a, b, p). The cases $u \notin \mathrm{nb}_U^{2^{m-i-1}}(\{a_1, \ldots, a_i\})$ and $v \notin \mathrm{nb}_V^{2^{m-i-1}}(\{b_1, \ldots, b_i\})$ are immediate from the assumption. $\diamondsuit$

Corollary 6.1 *If the set of all m-overlaps from U to V is an an m-neighbourhood system from U to V, then $U \equiv_m V$.* $\diamondsuit$

The following corollary is a strengthening of Hanf's Theorem.

Corollary 6.2 *If there is an m-sequence k to $\mathbb{N}$ such that for all $u \in \mathrm{dom}(U)$ and $0 \leq i < m$*

$$|\mathrm{nb}_{U}^{2^{m-i-1}}(u)| \leq k_i$$

and for each isomorphism type τ of a structure over $\mathrm{L} \cup \mathrm{C} \cup \{e\}$ either there are the same number of elements whose $2^{m-i-1} - 1$-neighbourhood type is τ in U and in V [4] *or in both $> ik_i$ elements with $2^{m-i-1} - 1$-neighbourhood type τ, then $U \equiv_m V$.*

Proof. Let $0 \leq i < m$ and $((a_1, \ldots, a_i), (b_1, \ldots, b_i), (p_1, \ldots, p_i))$ be an m-overlap from U to V. Set $A = \{a_1, \ldots, a_i\}$ $B = \{b_1, \ldots, b_i\}$. $|\mathrm{nb}_{U}^{2^{m-i-1}}(A)| \leq ik_i$. By Proposition 6.4 (b) $|\mathrm{nb}_{V}^{2^{m-i-1}}(B)| \leq ik_i$ and for each isomorphism type τ of a structure over $\mathrm{L} \cup \mathrm{C} \cup \{e\}$ there are the same number of elements in $\mathrm{nb}_{U}^{2^{m-i-1}}(A)$ of $2^{m-i-1} - 1$-neighbourhood type τ in U as of elements in $\mathrm{nb}_{V}^{2^{m-i-1}}(B)$ of $2^{m-i-1} - 1$-neighbourhood type τ in V. This means that condition (2) in the definition of n-neighbourhood system is fulfilled for the set of all m-overlaps from U to V. Corollary 6.1 now yields the claim. $\diamondsuit$

6.2 r, k-paths

In this section we apply Corollary 6.2 to rather simple structures, called r, k-paths. The results from this application will be used in Chapter 7 to construct an example for The-

[4] I. e. the number of $a \in \mathrm{dom}(U)$ whose $2^{m-i-1} - 1$-neighbourhood type in U is τ is equal to the number of $a \in \mathrm{dom}(V)$ whose $2^{m-i-1} - 1$-neighbourhood type in V is τ.

orem 7.7, which, in turn, will deliver, in Chapter 12, a result about the synthesizability from combinations of formulas.

Throughout this whole section and the next two sections 6.3, 6.4 let $c_0, c_1, \ldots$ be (distinct) constants, $\mathrm{C}_r = \{c_0, \ldots, c_{r-1}\}$ $(r \in \mathbb{N})$ and P, Q be (distinct) 1-placed relation symbols. A *k-path* $(k \in \mathbb{N})$ is an expansion U over $\{P, Q, R_1\}$ of a 1-multigraph (i. e. $U \upharpoonright \{R_1\}$ is a 1-multigraph) with $\mathrm{dom}(U) = \{a_0, \ldots, a_{k+1}\}$ for distinct $a_0, \ldots, a_{k+1}$, satisfying for all $0 \leq i \leq j \leq k+1$

$P^U(a_i)$ iff $i = 0$,

$Q^U(a_i)$ iff $i = k+1$,

$R_1^U(a_i, a_j)$ iff $j = i+1$.

Any two k-paths are obviously isomorphic. An *r, k-path* $(r, k \in \mathbb{N})$ is an expansion of a k-path with C_r. If U is an r, k-path, the element $u \in \mathrm{dom}(U)$ for which $P^U(u)$ respectively $Q^U(u)$ is called the *left* respectively the *right end point* of U and denoted by $\mathrm{lft}(U)$ respectively $\mathrm{rgt}(U)$. An *end point* of U is the left or the right end point of U.

Let U be an r, k-path. We define L_U: $\{0, \ldots, k+1\} \to \mathrm{dom}(U)$ by

$L_U(0) = \mathrm{lft}(U)$,

$L_U(i+1)$ is the $u \in \mathrm{dom}(U) \setminus \{L_U(0), \ldots, L_U(i-1)\}$ with $R_1^U(L_U(i), u)$ $(0 \leq i < k+1)$.

Furthermore we denote the inverse function L_U^{-1} of L_U by P_U and set $\mathrm{dst}_U(u, v) = |P_U(u) - P_U(v)|$ to be the absolute value of $P_U(u) - P_U(v)$ $(u, v \in \mathrm{dom}(U))$. The following proposition is easy to prove for all $u, v \in \mathrm{dom}(U)$ and $n \in \mathbb{N}$.

Proposition 6.6 $u \in \mathrm{nb}_U^n(v)$ iff $\mathrm{dst}_U(u, v) \leq n$. $\diamondsuit$

A *list* of U is an injective, thus a bijective, sequence $i_0, \ldots, i_{r-1}$ to $\{0, \ldots, r-1\}$ (usually also called a permutation of $\{0, \ldots, r-1\}$) for which $P_U(c_{i_0}^U) \leq \ldots \leq P_U(c_{i_{r-1}}^U)$. If i is a list of U, we call the sequence

$P_U(c_{i_0}^U), P_U(c_{i_1}^U) - P_U(c_{i_0}^U), \ldots, P_U(c_{i_{r-1}}^U) - P_U(c_{i_{r-2}}^U), k + 2 - P_U(c_{i_{r-1}}^U)$, if $r > 0$,

$k + 1$, if $r = 0$,

the *signature* of U. It is easy to verify that the signature of U is independent of the list that defines it. $u \in \mathrm{dom}(U)$ is called *n-isolated* in U ($n \in \mathbb{N}$) iff $c_i^U \notin \mathrm{nb}_U^n(u)$ for all $0 \leq i < r$, $\mathrm{lft}(U) \notin \mathrm{nb}_U^{n-1}(u)$ and $\mathrm{rgt}(U) \notin \mathrm{nb}_U^{n-1}(u)$ (define $\mathrm{nb}_U^{-1}(u) = \emptyset$).

Let $m, n, r, k, l \in \mathbb{N}$, $n \neq 0$, U be an r, k-path and V an r, l-path. U, V are called *n-distance equivalent* iff for all $0 \leq i, j < r$:

(i) $c_i^U \in \mathrm{nb}_U^h(c_j^U)$ iff $c_i^V \in \mathrm{nb}_V^h(c_j^V)$ ($h \leq n$).

(ii) $\mathrm{lft}(U) \in \mathrm{nb}_U^{h-1}(c_i^U)$ iff $\mathrm{lft}(V) \in \mathrm{nb}_V^{h-1}(c_i^V)$ ($0 < h \leq n$).

(iii) $\mathrm{rgt}(U) \in \mathrm{nb}_U^{h-1}(c_i^U)$ iff $\mathrm{rgt}(V) \in \mathrm{nb}_V^{h-1}(c_i^V)$ ($0 < h \leq n$).

(iv) $\mathrm{lft}(U) \in \mathrm{nb}_U^{h-2}(\mathrm{rgt}(U))$ iff $\mathrm{lft}(V) \in \mathrm{nb}_V^{h-2}(\mathrm{rgt}(V))$ ($1 < h \leq n$).

(iv) follows from (i) - (iii), if $r \geq 1$. Obviously, if U, V are n-distance equivalent, $U \equiv_0 V$ and, consequently, if $r \geq 1$, $U|\mathrm{C}_r^U \cong V|\mathrm{C}_r^V$.

Proposition 6.7 *If U, V are not 2^m-distance equivalent, then $U \not\equiv_m V$.*

Proof. First consider the case $r, m \geq 1$. Assume (a). Let W be an r,k-path whose signature p satisfies

$p_0 \geq 2^m$; $p_i \geq 2^m + 1$ $(0 < i \leq r)$.

W has a 2^{m-1}-isolated point, but no r,l-path that is 2^m-distance equivalent to W has one. Proposition 6.7 and Corollary 6.3 imply that no r,l-path is m-equivalent to W. Assume (b). Let W be an r,k-path whose signature p satisfies

$p_0 \leq 2^m$; $p_i \leq 2^m + 1$ $(0 < i \leq r)$.

W does not have a 2^{m-1}-isolated point, but every r,l-path that is 2^m-distance equivalent to W has one. Again, by Proposition 6.7 and Corollary 6.3, no r,l-path is m-equivalent to W.

The case $r = 0,\ m \geq 2$ is the case $r = 1,\ m - 1$. ♢

Theorem 6.2 *Assume $r, m \geq 1$ or $m \geq 2$. The k-path is r,m-equivalent to the l-path iff to every r,k-path there is an m-equivalent r,l-path iff $k = l$ or $k, l \geq 2^m(r+1)+r-x$.*

Proof. Follows from Lemma 6.1 and Lemma 6.2. ♢

Corollary 6.4 *If $r, m \geq 1$ or $m \geq 2$, then $2^m(r+1)+r-x$ is the smallest $n \in \mathbb{N}$ such that for all $k \geq n$ the k-path is r,m-equivalent to the n-path.* ♢

6.3 Connected sequences modulo k

$c_0, c_1, \ldots$, P and Q have been declared in the previous section. Motivated by the property of the shift operation, we define the r-sequence u to $\mathrm{dom}(U)$ *connected modulo k* in the structure U over the set L of relation symbols ($r, k \in \mathbb{N},\ k \geq 1$) iff k divides r (i. e. $r = ik$ for some $i \in \mathbb{N}$) and for all $0 \leq i < r/k$ the structure $U|\{u_{ik}, \ldots, u_{(i+1)k-1}\}$ is connected or $\{u_{ik}, \ldots, u_{(i+1)k-1}\} \subseteq \{u_0, \ldots, u_{ik-1}\}$.

Proposition 6.13 (a) *If k divides r, the r-sequence $v, \ldots, v$ ($v \in \mathrm{dom}(U)$) is connected modulo k in U.*

(b) *u is connected modulo 1 in U.* $\diamondsuit$

We refine the definition of r, m-equivalence given in the preliminaries. First we abbreviate $(U, (c_i\colon u_i)_{0 \leq i < r})$ by (U, u). Let U, V be structures over L. U, V are *k, r, m-equivalent* ($k, r, m \in \mathbb{N},\ k \geq 1$), $U \equiv_{k,r,m} V$, iff for all r-sequences u to $\mathrm{dom}(U)$ that are connected modulo k in U there is an r-sequence v to $\mathrm{dom}(V)$ and for all r-sequences v to $\mathrm{dom}(V)$ that are connected modulo k in V an r-sequence u to $\mathrm{dom}(U)$ with $(U, u) \equiv_m (V, v)$. Obviously $U \equiv_{1,r,m} V$ iff $U \equiv_{r,m} V$, because of Proposition 6.13 (b).

Proposition 6.14 *Assume that there is an r-sequence u to $\mathrm{dom}(U)$ connected modulo k in U and that $U \equiv_{k,r,m} V$. Then $U \equiv_{k,i,m} V$ for all $i \leq r$.*

Proof. If $r = 0$, the claim obviously holds. Let $r > 0$. From the assumption k divides r and, since $(U, u) \equiv_m (V, v)$ for some r-sequence v to $\mathrm{dom}(V)$, $U \equiv_m V$. Therefore the claim holds for $i = 0$. Assume $0 < i \leq r$. If k does not divide i, the claim trivially holds. Assume finally that k divides i and let w be an i-sequence to $\mathrm{dom}(U)$ that is connected modulo k in U. The r-sequence $\bar{w} = w_0, \ldots, w_{i-1}, w_0, \ldots, w_0$ is connected

(a) $k \geq 2^m(r/2+1)+r-x$ *and* $l < 2^m(r/2+1)+r-x$ *or*

(b) $k < 2^m(r/2+1)+r-x$ *and* $k \neq l$.

Then there is a shift r,k-path to which no r,l-path is m-equivalent (which implies that the k-path is not $2,r,m$-equivalent to the l-path).

Proof. First consider the case $r,m \geq 1$. Assume (a). Let W be an r,k-path whose signature p satisfies

$$p_0 \geq 2^m;\ p_{2i} \geq 2^m+1\ (0 < i \leq r/2);\ p_{2i+1} = 1\ (0 \leq i < r/2).$$

W has a 2^{m-1}-isolated point, but no r,l-path that is 2^m-distance equivalent to W has one. Proposition 6.7 and Corollary 6.3 imply that no r,l-path is m-equivalent to W. Assume (b). Let W be an r,k-path whose signature p satisfies

$$p_0 \leq 2^m;\ p_{2i} \leq 2^m+1\ (0 < i \leq r/2);\ p_{2i+1} = 1\ (0 \leq i < r/2).$$

W does not have a 2^{m-1}-isolated point, but every r,l-path that is 2^m-distance equivalent to W has one. Again, by Proposition 6.7 and Corollary 6.3, no r,l-path is m-equivalent to W.

The case $r=0,\ m \geq 2$ is the case $r=1,\ m-1$. ♢

Theorem 6.3 *Assume $r,m \geq 1$ or $m \geq 2$. The k-path is $2,r,m$-equivalent to the l-path iff to every shift r,k-path there is an m-equivalent r,l-path iff $k=l$ or $k,l \geq 2^m(r/2+1)+r-x$.*

Proof. Follows from Lemma 6.3 and Lemma 6.4. ♢

Corollary 6.5 *If $r, m \geq 1$ or $m \geq 2$, then $2^m(r/2+1)+r-x$ is the smallest $n \in \mathbb{N}$ such that for all $k \geq n$ the k-path is $2, r, m$-equivalent to the n-path.* $\diamondsuit$

6.4 Alternate k-paths and $\langle l, k\rangle$-paths

In this section we introduce two variants of a k-path and investigate them briefly in the light of the results obtained for k-paths. The conclusions of this investigation will be used in Chapter 7 to construct more examples for Theorem 7.7 (k-paths will be used for this purpose, too). All these examples will deliver, in Chapter 12, a result about the synthesizability from combinations of formulas. It should be pointed out that, to the contrary of what was done for the k-paths, we will not characterize up to the last detail neither the r, m- nor the $2, r, m$-equivalence between these variants of the k-paths, but limit ourself to the statements needed for the examples we will construct from them.

$c_0, c_1, \ldots, \mathrm{C}_r$ ($r \in \mathbb{N}$) and P, Q have been set in Section 6.2. Throughout this whole section let $S(\neq P, Q)$ be a 1-placed relation symbol. An *alternate k-path* ($k \in \mathbb{N}$) is an expansion U over $\{P, Q, R_1, R_2\}$ of a 2-multigraph with $\mathrm{dom}(U) = \{a_0, \ldots, a_{k+1}\}$ for distinct $a_0, \ldots, a_{k+1}$, satisfying for all $0 \leq i \leq j \leq k+1$

$P^U(a_i)$ iff $i = 0$,

$Q^U(a_i)$ iff $i = k+1$,

$R_1^U(a_i, a_j)$ iff $j = i+1$ and i is even,

$R_2^U(a_i, a_j)$ iff $j = i+1$ and i odd.

Any two alternate k-paths are obviously isomorphic. An *alternate r, k-path* ($r, k \in \mathbb{N}$)

is an expansion of an alternate k-path with C_r. An *alternate shift* r,k*-path* $(r,k \in \mathbb{N})$ as an alternate r,k-path U for which $c_0^U, \ldots, c_{r-1}^U$ is connected modulo 2 in U.

Let $m,n,r,k,l \in \mathbb{N}$, $n \neq 0$. We define, for an alternate r,k-path U and an alternate r,l-path V, $\mathrm{lft}(U)$, $\mathrm{rgt}(U)$, $u \in \mathrm{dom}(U)$ n*-isolated* in U, U,V n*-distance equivalent* and P_U exactly as we did for r,k-paths, where L_U: $\{0,\ldots,k+1\} \to \mathrm{dom}(U)$ is given by

$L_U(0) = \mathrm{lft}(U)$,

$L_U(i+1)$ is the $u \in \mathrm{dom}(U) \setminus \{L_U(0),\ldots,L_U(i-1)\}$ with $R_1^U(L_U(i),u)$ or $R_2^U(L_U(i),u)$ $(0 \leq i < k+1)$.

Let again U be an alternate r,k-path and V an alternate r,l-path. We define U,V *congruent* iff

k is even iff l is even and for all $0 \leq i,j < r$

$P_U(c_i^U)$ is even iff $P_V(c_i^V)$ is even and

if $P_U(c_i^U) \leq P_U(c_j^U)$, then $P_V(c_i^V) \leq P_V(c_j^V)$.

If U,V are congruent, it still holds, as it did for r,k-paths, that if they are n-distance equivalent, then $U \equiv_0 V$, whence $U|\mathrm{C}_r^U \sim V|\mathrm{C}_r^V$.

Suppose that f is an isomorphism from $U \restriction \{R_1,R_2\}|\mathrm{nb}_U^n(u)$ to $V \restriction \{R_1,R_2\}|\mathrm{nb}_V^n(v)$ with $f(u) = v$ such that for all $0 \leq i < r$

if $c_i^U \in \mathrm{nb}_U^n(u)$, $f(c_i^U) = c_i^V$,

if $\mathrm{lft}(U) \in \mathrm{nb}_U^{n-1}(u)$, $f(\mathrm{lft}(U)) = \mathrm{lft}(V)$,

if $\mathrm{rgt}(U) \in \mathrm{nb}_U^{n-1}(u)$, $f(\mathrm{rgt}(U)) = \mathrm{rgt}(V)$.

Set $\bar{f}$ with $\mathrm{dom}(\bar{f}) = \mathrm{dom}(U^n(u))$ by $\bar{f} \supseteq f$ and $\bar{f}(c_i^U) = c_i^V$ for all $0 \leq i < r$. Then

7 Interpretations

Interpretations are fundamental in the mathematical way of thinking. They allow to perceive a structure to be (essentially) the same as another one, in spite of appearing different. For example it is well known that through one interpretation every boolean ring transforms into a boolean algebra and every boolean algebra is that interpretation of a boolean ring (refer in this regard for example to [1]). This implies (with Theorem 7.4) that an expert in the (first-order) theory of rings is also an expert in the theory of boolean algebras.

In Chapter 7 interpretations are defined and investigated under the aspects that are relevant for the application to synthesizability. Subsequently, in Chapter 10, they are narrowed down to reactional interpretations, which, on n-multigraphs, are equivalent to $\mathcal{S}$-shifts (with $\mathcal{S}$ a finite set of finite n-rules). $\mathcal{S}$-shifts are the inspiring force behind our study of interpretations, which, in this book, are seen as a generalization of the $\mathcal{S}$-shift operation and therefore considered to play an important role in the study and the understanding of synthesizability.

Reactional interpretations are a particular case of regular interpretations, also introduced in Chapter 10. The name "regular" has been chosen because of its derivation from the latin word "regula" (in english: "rule"). Regular interpretations are quantifier-free. Therefore a particular emphasis is put, in the initial part of this chapter, on quantifier-free interpretations. From the considerations above it is clear, in spite of their apparent simplicity, that they are plenty powerful enough to express all the synthesizability problems defined in Chapter 3.

The iteration of an interpretation is achieved, naturally, through the composition of interpretations, which is examined in Section 7.1. The composition of interpretations leads to the definitions of rank and bound, which play a key role in establishing the axiomatizability of the class of structures that can be obtained through an iteration (finitely many times) of the interpretation, starting with the models of a sentence.

This book attempts to shed some light on the class $\vec{\varphi}(\mathcal{C})$ of structures obtained by applying an interpretation φ finitely many times to a structure in an initial class $\mathcal{C}$, on the basis of the properties of $\mathcal{C}$, i. e. on which (preservation) properties $\mathbf{P}, \mathbf{Q}$ satisfy the condition that $\mathbf{Q}$ is true for $\vec{\varphi}(\mathcal{C})$, if $\mathbf{P}$ is true for $\mathcal{C}$. Said differently, on which properties of $\mathcal{C}$ translate into a corresponding property of $\vec{\varphi}(\mathcal{C})$. It is, for example, a simple result of this chapter that preservation under isomorphisms translate into itself (i. e. if $\mathcal{C}$ has it, so does $\vec{\varphi}(\mathcal{C})$). While the set $\varphi(\mathcal{C})$ of the structures that φ interprets in a structure in $\mathcal{C}$ is preserved under ultraproducts, if $\mathcal{C}$ is (Theorem 7.1), $\vec{\varphi}(\mathcal{C})$ is not necessarily preserved under ultraproducts, not even if $\mathcal{C}$ is axiomatized by a sentence (Corollary 10.2).

If φ is a quantifier-free interpretation for a finite set of relations symbols of range 0, Proposition 7.18 states that also the preservation under chains (which is short for preservation under unions of chains) translates into itself. This subject will be treated more extensively in Chapter 9.

On our way to the regular interpretations, we meet, in Section 7.3, the weakly invertible and invertible interpretations. As the name says, invertible interpretations are a particular case of weakly invertible interpretations, being the definition of the latter weaker than the definition of the former. Interestingly, though, by Corollary 7.30, there are no strictly weakly invertible, quantifier-free interpretations of range 0 for a finite set of relations symbols.

In Section 7.3, as in the initial part of this chapter, we put a special emphasis on quantifier-free interpretations and prove that, if they are weakly invertible, their inverse is itself quantifier-free. For a quantifier-free, invertible interpretation φ of range 0 for a finite set of relations symbols we mention two more properties, namely preservation under i-sandwiches and under i-fillings, which translate into themselves, when passing from a class $\mathcal{C}$ to $\vec{\varphi}(\mathcal{C})$.

In Section 7.2 we draw some conclusions under the condition that an interpretation is iterated a fixed (but, of course, arbitrary) finite number of times and the underlying set of symbols is finite. Given our inspiration source of the study of interpretations, which is the $\mathcal{S}$-shift, we specify interpretations through the graph theoretical definition of interpretation connected modulo a natural number. The conclusions in Section 7.2 lead to surprisingly low upper bounds for the size of a combination of a set of structures, to which an application of an interpretation a fixed, finite number of times yields a model of a sentence, if such a combination exists.

In Section 7.3 these conclusions are merged with the results of Chapter 6, delivering the explicit calculations for two rather simple but emblematic classes, that will provide the material for yet more concrete examples in Chapter 12.

Before beginning the discussion about interpretations we choose (distinct) constant symbols $c_0, c_1, \ldots$ If L is a set of relation symbols, we denote by L_r the set $\mathrm{L} \cup \{c_0, \ldots, c_{r-1}\}$ and, for a structure U over L and an r-sequence u to $\mathrm{dom}(U)$, by (U, u) the expansion $(U, (c_i : u_i)_{0 \leq i < r})$ of U.

An *interpretation* for the set L of relation symbols of *range* $r \in \mathbb{N}$ is a mapping

$$(\varphi_R(x_0, \ldots, x_{\nu_R - 1}))_{R \in \mathrm{L}},$$

where φ_R is a formula in L_r for every $R \in \mathrm{L}$. In order to have the range uniquely determined we require that for some $R \in \mathrm{L}$ the constant c_{r-1} occurs in φ_R, if $r > 0$. An *interpretation* for L is an interpretation for L of some range and an *interpretation* is an interpretation for some set of relation symbols.

Let L be a set of relation symbols.

The interpretation $(\varphi_R)_{R \in \mathrm{L}}$ is called *quantifier-free* iff φ_R is quantifier-free for all $R \in \mathrm{L}$.

The interpretation ω^{L} for L of range 0 given by

$$\omega^{\mathrm{L}}_R \;=\; R x_0 \ldots x_{\nu_R - 1}$$

for all $R \in \mathrm{L}$ is called the *identity interpretation* for L. φ is called *quantifier bound* iff there is $k \in \mathbb{N}$ such that $\mathrm{qr}(\varphi_R) < k$ for all $R \in \mathrm{L}$. If φ is quantifier bound we define $\mathrm{qr}(\varphi)$, the *quantifier rank* of φ, as follows:

$$\mathrm{qr}(\varphi) = \begin{cases} \max\{\mathrm{qr}(\varphi_R) \mid R \in \mathrm{L}\} & \text{if } \mathrm{L} \neq \emptyset; \\ 0 & \text{if } \mathrm{L} = \emptyset. \end{cases}$$

Let φ be an interpretation for L of range r and $s \geq r$.

If U is a structure over L_s, $\varphi(U)$ is the structure V over L_{s-r} with $\mathrm{dom}(V) = \mathrm{dom}(U)$ and $c_i^V = c_{r+i}^U$ $(0 \leq i < s-r)$, satisfying for all $R \in \mathrm{L}$ and all ν_R-sequences u to $\mathrm{dom}(U)$

$$R^V(u_0, \ldots, u_{\nu_R-1}) \text{ iff } U \models \varphi_R[u].$$

Consequently, for a structure U over L and an s-sequence u to $\mathrm{dom}(U)$,

$$\varphi(U, u) = (\varphi(U, u_0, \ldots, u_{r-1}), u_r, \ldots, u_{s-1}).$$

For structures U, V over L, φ *carries* U into V at the r-sequence u to $\mathrm{dom}(U)$ iff $V = \varphi(U, u)$. φ *carries* U into V iff φ carries U into V at some r-sequence u to $\mathrm{dom}(U)$. Instead of writing that φ carries U into V (at u), we might write that φ *defines* or *interprets* V in U (at u). For a class $\mathcal{C}$ of structures over L we define $\varphi(\mathcal{C})$ to be the class of all structures that φ defines in some $U \in \mathcal{C}$. For a structure U over L, instead of writing $\varphi(\{U\})$ we will write $\varphi(U)$. The proof of the next proposition is straightforward.

Proposition 7.1 *If φ is quantifier-free and $V \subseteq U$ are structures over L_s, then $\varphi(V) \subseteq \varphi(U)$.* $\diamondsuit$

The interpretations ϕ, ψ for L of range r are *equivalent*, $\phi \leftrightarrow \psi$, iff $\phi(U) = \psi(U)$ for all structures U over L_r. $\leftrightarrow$ is obviously an equivalence relation over the set of all interpretations for L. We will not distinguish between ϕ and the equivalence class $[\phi]_\leftrightarrow$ of ϕ modulo $\leftrightarrow$.

Proof. (a) First assume $(U,u) \models \gamma$. Choose an $(r+s)$-sequence $\bar{u}$ extending u with $(U,\bar{u}) \models \delta$. We have $R^{(\varphi|\gamma)(U,u)}(a_0,\dots,a_{\nu_R-1})$ iff $(U,u) \models (\varphi|\gamma)_R[a_0,\dots,a_{\nu_R-1}]$ iff $(U,u) \models \varphi_R[a_0,\dots,a_{\nu_R-1}]$ iff $(U,\bar{u}) \models \varphi_R[a_0,\dots,a_{\nu_R-1}]$ iff $(U,\bar{u}) \models (\varphi|\delta)_R[a_0,\dots,a_{\nu_R-1}]$ iff $R^{(\varphi|\delta)(U,\bar{u})}(a_0,\dots,a_{\nu_R-1})$. If $(U,u) \not\models \gamma$, choose any extension $\bar{u}$ of u and proceed analogously to the first part.

(b) Assume $\varphi(U,v) = U$ for the r-sequence v to $\mathrm{dom}(U)$ and let $\bar{u}$ be a $(r+s)$-sequence to $\mathrm{dom}(U)$. If $(U,\bar{u}) \models \delta$, choose $u_0,\dots,u_{r-1}$, otherwise (i. e. if $(U,\bar{u}) \not\models \delta$) choose v. In the first case the calculation is analogous to the one in the first part of (a), since $(U,\bar{u}) \models \delta$ implies $(U,u) \models \gamma$. The calculation for the second case looks as follows: $R^{(\varphi|\gamma)(U,v)}(a_0,\dots,a_{\nu_R-1})$ iff $(U,v) \models (\varphi|\gamma)_R[a_0,\dots,a_{\nu_R-1}]$ iff $(U,v) \models ((\gamma \to \varphi_R) \wedge (\neg\gamma \to Rx_0\dots x_{\nu_R-1}))[a_0,\dots,a_{\nu_R-1}]$ iff

$(U,v) \models \gamma$ and $(U,v) \models \varphi_R[a_0,\dots,a_{\nu_R-1}]$ or

$(U,v) \not\models \gamma$ and $(U,v) \models Rx_0\dots x_{\nu_R-1}[a_0,\dots,a_{\nu_R-1}]$ iff

$(U,v) \models \gamma$ and $(U,v) \models Rx_0\dots x_{\nu_R-1}[a_0,\dots,a_{\nu_R-1}]$ or

$(U,v) \not\models \gamma$ and $(U,v) \models Rx_0\dots x_{\nu_R-1}[a_0,\dots,a_{\nu_R-1}]$ iff

$(U,v) \models Rx_0\dots x_{\nu_R-1}[a_0,\dots,a_{\nu_R-1}]$ iff $(U,\bar{u}) \models Rx_0\dots x_{\nu_R-1}[a_0,\dots,a_{\nu_R-1}]$ iff $(U,\bar{u}) \models (\varphi|\delta)_R[a_0,\dots,a_{\nu_R-1}]$ iff $R^{(\varphi|\delta)(U,\bar{u})}(a_0,\dots,a_{\nu_R-1})$. $\diamondsuit$

The class of all structures U over L_r with $\varphi(U) \neq U \restriction \mathrm{L}$ is called the *domain* of φ, $\mathrm{dom}(\varphi)$. We set

$$\zeta_\varphi = \bigvee_{R \in \mathrm{L}} \exists x_0 \dots x_{\nu_r-1} \neg(Rx_0\dots x_{\nu_r-1} \leftrightarrow \varphi_R).$$

Proposition 7.4 *ζ_φ axiomatizes* $\mathrm{dom}(\varphi)$ *(i. e. $U \models \zeta_\varphi$ iff $\varphi(U) \neq U \restriction \mathrm{L}$ for every structure U over L_r).*

Proof. Straightforward. $\diamondsuit$

Let $\mathcal{C}$ be a class of structures over L closed under isomorphisms.

Proposition 7.5 *The class $\varphi(\mathcal{C})$ is closed under isomorphisms.*

Proof. Let $U \in \mathcal{C}$, u be an r-sequence to $\mathrm{dom}(U)$ and f be an isomorphism from V to $\varphi(U, u)$. Define U' to be the structure from which f is an isomorphism to U. $U' \in \mathcal{C}$. Then for all $v_0, \ldots, v_{\nu_R-1} \in \mathrm{dom}(V)$

$R^V(v_0, \ldots, v_{\nu_R-1})$ iff $(U, u) \models \varphi_R[f(v_0), \ldots, f(v_{\nu_R-1})]$ iff

$(U', f^{-1}(u_0), \ldots, f^{-1}(u_{r-1})) \models \varphi_R[v_0, \ldots, v_{\nu_R-1}]$ iff

$R^{\varphi(U', f^{-1}(u_0), \ldots, f^{-1}(u_{r-1}))}(v_0, \ldots, v_{\nu_R-1})$.

Hence $V = \varphi(U', f^{-1}(u_0), \ldots, f^{-1}(u_{r-1}))$, which implies $V \in \varphi(\mathcal{C})$. $\diamondsuit$

It follows from the next Theorem 7.1 that, if a class $\mathcal{C}$ of structures over L is closed under ultraproducts, then so is the class $\varphi(\mathcal{C})$ of all structures that φ defines in a structure of $\mathcal{C}$. The main facts about ultrafilters and ultraproducts can be found in [5], [6], [7]. Let $\mathcal{F}$ be an ultrafilter over the set I. $\mathcal{F}$ is seen as an equivalence relation over the class of all functions with domain I ($f \equiv_{\mathcal{F}} g$ iff $\{i \in I \mid f(i) = g(i)\} \in \mathcal{F}$). If A_i is a set and U_i a structure over L for all $i \in I$, we denote by $\prod(A_i)_{i\in I}$, $\prod(A_i)_{i\in I}/\mathcal{F}$, $\prod(U_i)_{i\in I}/\mathcal{F}$ respectively the direct product of $(A_i)_{i\in I}$, the ultraproduct modulo $\mathcal{F}$ of $(A_i)_{i\in I}$ and the ultraproduct modulo $\mathcal{F}$ of $(U_i)_{i\in I}$.

Let U_i be a structure over L for all $i \in I$ and $u_0, \ldots, u_{r-1} \in \prod(\mathrm{dom}(U_i))_{i\in I}$, i. e. $u_{ji} \in \mathrm{dom}(U_i)$ for all $0 \leq j < r$, $i \in I$. For $v \in \prod(\mathrm{dom}(U_i))_{i\in I}$ let $[v]_{\prod(U_i)_{i\in I}/\mathcal{F}}$ be the element of $\mathrm{dom}(\prod(U_i)_{i\in I}/\mathcal{F})$ to which v belongs, i. e. the class $A \in \prod(\mathrm{dom}(U_i))_{i\in I}/\mathcal{F}$ with $v \in A$. To simplify the notation we just write $[v]$ instead of $[v]_{\prod(U_i)_{i\in I}/\mathcal{F}}$.

Theorem 7.1

$$\varphi(\prod(U_i)_{i\in I}/\mathcal{F}, [u_0], \ldots, [u_{r-1}]) = \prod(\varphi(U_i, u_{0i}, \ldots, u_{(r-1)i}))_{i\in I}/\mathcal{F}.$$

Proof. Let $R \in \mathrm{L}$, $v_0, \ldots, v_{\nu_R-1} \in \prod(\mathrm{dom}(U_i))_{i\in I}/\mathcal{F}$.

$$\begin{array}{ll}
R^{\varphi(\prod(U_i)_{i\in I}/\mathcal{F}, [u_0], \ldots, [u_{r-1}])}([v_0], \ldots, [v_{\nu_R-1}]) & \text{iff} \\
(\prod(U_i)_{i\in I}/\mathcal{F}, [u_0], \ldots, [u_{r-1}]) \models \varphi_R[[v_0], \ldots, [v_{\nu_R-1}]] & \text{iff} \\
\prod(U_i, u_{0i}, \ldots, u_{(r-1)i})_{i\in I}/\mathcal{F} \models \varphi_R[[v_0], \ldots, [v_{\nu_R-1}]] & \text{iff} \\
\{i \in I \mid (U_i, u_{0i}, \ldots, u_{(r-1)i}) \models \varphi_R[v_{0i}, \ldots, v_{(\nu_R-1)i}]\} \in \mathcal{F} & \text{iff} \\
\{i \in I \mid R^{\varphi(U_i, u_{0i}, \ldots, u_{(r-1)i})}(v_{0i}, \ldots, v_{(\nu_R-1)i})\} \in \mathcal{F} & \text{iff} \\
R^{\prod(\varphi(U_i, u_{0i}, \ldots, u_{(r-1)i}))_{i\in I}/\mathcal{F}}([v_0], \ldots, [v_{\nu_R-1}]). &
\end{array}$$

The third equivalence is implied by the Theorem of Łoś. $\diamondsuit$

Let T be a theory in L. We are now in the position of stating two necessary and sufficient conditions for $\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$ to be first-order axiomatizable.

Theorem 7.2 $\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$ *is first-order axiomatizable iff it is closed under elementary equivalence iff for every structure U over* L*, if some ultrapower of U is in* $\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$*, so is U.*

The following Corollary 7.2 (of Corollary 7.1) can be proven analogously to Corollary 3.1.

Corollary 7.2 *Let $\mathcal{U}$ be a set of structures over* L *with pairwise disjoint domains. Assume φ is quantifier-free. V is a (k-step) φ-product of a combination of $\mathcal{U}$ iff it is a (k-step) φ-product of a combination of $\sum\mathcal{U}$. If $\mathcal{U}$ is finite, then V is a (k-step) φ-product of a finite-combination of $\mathcal{U}$ iff it is a (k-step) φ-product of a finite-combination of $\sum\mathcal{U}$.* $\diamondsuit$

Let $\mathcal{C}$ be a class of structures over L. The proofs of the following two propositions, that will be used later in Chapter 9, are immediate.

Proposition 7.6 *The sentence δ in* L *is φ-derivable from a structure in $\mathcal{C}$ iff $\neg\delta \notin$* $\mathrm{Th}(\vec{\varphi}(\mathcal{C}))$. $\diamondsuit$

Proposition 7.7 *If the theory* T *in* L *axiomatizes $\vec{\varphi}(\mathcal{C})$, then* T *axiomatizes $\vec{\varphi}(\mathcal{C}^{\mathrm{f}})$ in the finite.*

Proof. Consequence of $\vec{\varphi}(\mathcal{C}^{\mathrm{f}}) = \vec{\varphi}(\mathcal{C})^{\mathrm{f}}$. $\diamondsuit$

Assume that L is finite and let Σ be a decidable set of sentences in L. The *φ-derivability* problem for $\mathcal{C}$, Σ is the question:

Given δ in Σ, is δ φ-derivable from a structure in $\mathcal{C}$ (i. e. is it consistent with $\vec{\varphi}(\mathcal{C})$)?

The φ-derivability problems (for $\mathcal{C}, \Sigma$) do not reflect accurately the synthesizability problems defined in Chapter 3. On one hand we will be interested exclusively in classes of structures $\mathrm{cmb}(\mathcal{U})$ for a finite set $\mathcal{U}$ of finite structures. On the other hand we want to have the possibility of a variable input for $\mathcal{U}$. For these reasons we introduce the φ-synthesizability problems.

Let this time $\mathcal{C}_0$ be a decidable class of finite sets of finite structures over L and $\mathcal{C}_1$ a decidable class of finite structures over L (both $\mathcal{C}_0$ and $\mathcal{C}_1$ closed under isomorphism [5]). The *φ-synthesizability* problem for $\mathcal{C}_0$, $\mathcal{C}_1$ is the question:

Given $U \in \mathcal{C}_1$ and $\mathcal{U} \in \mathcal{C}_0$, is U a φ-product of a combination of $\mathcal{U}$?

The *elementary φ-synthesizability* problem for $\mathcal{C}_0$, Σ is the question:

Given δ in Σ and $\mathcal{U} \in \mathcal{C}_0$, is δ φ-derivable from a combination of $\mathcal{U}$?

We will omit $\mathcal{C}_1$ in the definition above, if $\mathcal{C}_1$ is the class of all the finite structures over L and Σ, in the definition above, if it is the set of all sentences in L. We simplify the notation, as we did for the synthesizability definition in Section 3.2, by assigning to $\mathcal{C}_1$ respectively $\mathcal{C}_0$ the value X for the class of all structures respectively finite sets of structures isomorphic to X and to Σ the value δ instead of $\{\delta\}$.

It follows immediately that the φ-derivability problem for $\mathrm{cmb}(\mathcal{U})$ and the elementary φ-synthesizability problem for $\mathcal{U}$ coincide.

Corollary 7.3 *The φ-derivability problem for $\mathcal{C}_0$ is solvable iff $\mathrm{Th}(\vec{\varphi}(\mathcal{C}_0))$ is decidable.*

Proof. Direct consequence of Proposition 7.6. $\diamondsuit$

Interpretations are introduced for example in [2]. Following the formalism in [2] we define Γ by the following items:

[5] The finite sets $\mathcal{U}, \mathcal{V}$ of structures over L are *isomorphic* iff for every $U \in \mathcal{U}$ there is $V \in \mathcal{V}$ with $U \cong V$ and vice versa.

$$\partial_\Gamma = \ x_0{=}x_0;$$

$$\phi_\Gamma = \begin{cases} \phi & \text{for } \phi = \ y{=}z \text{ and variables } y, z; \\ c_{r+i}{=}y & \text{for } \phi = \ c_i{=}y \ \ (0 \leq i < s-r \text{ and variable } y); \\ \varphi_R(y_0, \ldots, y_{\nu_R-1}) & \text{for } \phi = \ Ry_0 \ldots y_{\nu_R-1} \text{ and variables } y_0, \ldots, y_{\nu_R-1}; \end{cases}$$

$$f_\Gamma = \ \mathrm{id}_{\,\mathrm{dom}(U)}.$$

Then Γ is an interpretation of $\varphi(U)$ in U for all structures U over L_s, i. e. for every $n \in \mathbb{N}$, every ϕ that is an atomic formula $\phi(x_0, \ldots, x_{n-1})$ in L or an atomic formula $\phi = \ c_i{=}x_j \ \ (0 \leq i < s-r, \ 0 \leq j < n)$ and all n-sequences u to $\mathrm{dom}(U)$ with $U \models \partial_\Gamma[u_i]$ $(0 \leq i < n)$

$$\varphi(U) \models \phi[f_\Gamma(u_0), \ldots, f_\Gamma(u_{n-1})] \text{ iff } U \models \phi_\Gamma[u_0, \ldots, u_{n-1}].$$

We now dedicate some attention to a class of interpretations that play a central role in this book: quantifier-free interpretations for a finite set of relation symbols. As a result we completely characterize this class. In Section 10.2 we will further restrict our investigation to quantifier-free, local interpretations, obtaining an even more simple characterization.

Let $\mathrm{L} \neq \emptyset$ be a finite set of relation symbols, $r \in \mathbb{N}$, $m = \max\{\nu_R \,|\, R \in \mathrm{L}\}$ and $\mathcal{U}$ the set of all structures over L_r whose domain is $\{0, \ldots, i\}$ $(0 \leq i < m+r)$. A function $F\colon \mathcal{U} \to \mathcal{U}$ is called *monotonic* iff $c_i^{F(U)} = c_i^U$ for all $0 \leq i < r$ and g is an embedding from $F(U)$ into $F(V)$ for all $U, V \in \mathcal{U}$ and all embeddings g from U into V. Assume that F is monotonic and $U, V \in \mathcal{U}$.

Proof. Let $F\colon \mathcal{U} \to \mathcal{U}$ be monotonic. G with $G(U) = (\Phi^F(U), c_0^U, \ldots, c_{r-1}^U)$ (U structure over L_r) as a consequence of Proposition 7.12 is an extension of F, that satisfies the condition in the definition of $\overline{F}$. Therefore $\overline{F} = G$. ♢

Theorem 7.3 completely characterizes the quantifier-free interpretations for a finite set of relation symbols.

Theorem 7.3 *The interpretation φ for* L *of range r is quantifier-free iff there is a monotonic $F\colon \mathcal{U} \to \mathcal{U}$ with $(\varphi(U), c_0^U, \ldots, c_{r-1}^U) = \overline{F}(U)$ for all structures U over L_r.*

Proof. Assume that φ is quantifier-free. E^φ is monotonic. By Lemma 7.1

$$(\varphi(U), c_0^U, \ldots, c_{r-1}^U) = \overline{E^\varphi}(U)$$

for all structures U over L_r. Assume that there is a monotonic $F\colon \mathcal{U} \to \mathcal{U}$ such that $(\varphi(U), c_0^U, \ldots, c_{r-1}^U) = \overline{F}(U)$ for all structures U over L_r. By Corollary 7.5 $\overline{F}(U) = (\Phi^F(U), c_0^U, \ldots, c_{r-1}^U)$ for all structures U over L_r. Thus $\varphi \leftrightarrow \Phi^F$. Since Φ^F is quantifier-free and we do not distinguish between φ and Φ^F, φ is quantifier-free. ♢

Proposition 7.13 *Assume that F is injective and F^{-1} monotonic. Then*

$$\Phi^F(\Phi^{F^{-1}}(U), c_0^U, \ldots, c_{r-1}^U) = \Phi^{F^{-1}}(\Phi^F(U), c_0^U, \ldots, c_{r-1}^U) = U \restriction \mathrm{L}$$

for all structures U over L_r.

Proof.

$$\Phi^F(\Phi^{F^{-1}}(U), c_0^U, \ldots, c_{r-1}^U) \overset{\text{Corollary 7.5}}{=} \overline{F}(\Phi^{F^{-1}}(U), c_0^U, \ldots, c_{r-1}^U) \restriction \mathrm{L} \overset{\text{Corollary 7.5}}{=}$$
$$\overline{F}(\overline{F^{-1}}(U)) \restriction \mathrm{L} \overset{\text{Proposition 7.11}}{=} U \restriction \mathrm{L}.$$

Same for $\Phi^{F^{-1}}(\Phi^F(U), c_0^U, \ldots, c_{r-1}^U)$. $\diamondsuit$

Proposition 7.14 *Assume that there is a quantifier-free interpretation* ψ *for* L *of range* r *with* $\Phi^F(\psi(U), c_0^U, \ldots, c_{r-1}^U) = U \restriction \mathrm{L}$ *for all structures* U *over* L_r. *Then* F *is injective and* F^{-1} *monotonic.*

Proof. By Lemma 7.1 $\Phi^F(\overline{E^\psi}(U)) = U \restriction \mathrm{L}$, whence, by Corollary 7.5, $\overline{F}(\overline{E^\psi}(U)) = U$, for all structures U over L_r. Therefore $F(E^\psi(U)) = U$ for all $U \in \mathcal{U}$. Since $\mathcal{U}$ is finite, F is injective and $F^{-1} = E^\psi$ monotonic. $\diamondsuit$

With Proposition 7.14 we conclude for the moment our discussion regarding quantifier-free interpretations and turn our attention to the iteration of interpretations.

7.1 Composition of interpretations

For the whole section let L be a set of relation symbols.

Let $\delta(x_0, \ldots, x_{m-1})$ be a formula in L_s $(m, s \in \mathbb{N})$ and φ an interpretation for L of range r. δ, φ are *composable* iff no variable in δ (free or not) occurs bound in any φ_R for all $R \in \mathrm{L}$. $\delta\,\varphi$ is obtained by replacing every subformula $Rt_0 \ldots t_{\nu_R-1}$ in $\delta[c_0, \ldots, c_{s-1} : c_r, \ldots, c_{r+s-1}]$ with $\varphi_R[t_0, \ldots, t_{\nu_R-1}]$:

$$\delta\,\varphi = \delta[c_0, \ldots, c_{s-1} : c_r, \ldots, c_{r+s-1}][\quad Rt_0 \ldots t_{\nu_R-1} : \varphi_R[t_0, \ldots, t_{\nu_R-1}]$$
$$(t_0, \ldots, t_{\nu_R-1} \text{ terms in } \{c_r, \ldots, c_{r+s-1}\}, R \in \mathrm{L}) \quad].$$

Theorem 7.4 *Assume that* δ, φ *are composable. Let* U *be a structure over* L_t $(t \geq r+s)$

and u be an m-sequence to $\mathrm{dom}(U)$*.*

$$U \models (\delta\,\varphi)\,[u] \textit{ iff } \varphi(U) \models \delta[u].$$

Proof. The proof is by induction on the construction of a formula. Suppose $\delta = Rt_0 \ldots t_{\nu_R-1}$.

$U \models (\delta\,\varphi)\,[u]$ iff

$U \models \varphi_R[t_0[c_0, \ldots, c_{s-1} : c_r, \ldots, c_{r+s-1}], \ldots, t_{\nu_R-1}[c_0, \ldots, c_{s-1} : c_r, \ldots, c_{r+s-1}]][u]$ iff

[since no variable in $t_0, \ldots, t_{\nu_R-1}$ occurs bound in φ_R]

$U \models \varphi_R[(t_0[c_0, \ldots, c_{s-1} : c_r, \ldots, c_{r+s-1}])^U[u], \ldots, (t_{\nu_R-1}[c_0, \ldots, c_{s-1} : c_r, \ldots, c_{r+s-1}])^U[u]]$ iff

$U \models \varphi_R[t_0^{\varphi(U)}[u], \ldots, t_{\nu_R-1}^{\varphi(U)}[u]]$ iff

$\varphi(U) \models Rt_0 \ldots t_{\nu_R-1}[u]$ iff

$\varphi(U) \models \delta[u]$.

The induction steps for $\wedge$ and $\neg$ are straightforward. Assume $\delta = \exists z\gamma$.

$U \models (\exists z\gamma)\,\varphi\,[u]$	iff
$U \models \exists z(\gamma\,\varphi)\,[u]$	iff
there is $v \in \mathrm{dom}(U)$ with $U \models \gamma\,\varphi\,[u, z : v]$	iff [by induction hypothesis]
there is $v \in \mathrm{dom}(U)$ with $\varphi(U) \models \gamma[u, z : v]$	iff
$\varphi(U) \models \delta[u]$.	

In the induction step above we followed the convention for $[u, z : v]$ that the assignment to a variable is given by its last occurrence in the assignment's sequence. $\diamondsuit$

Let φ be an interpretation for L of range r. A theory T in L is *closed* under φ iff $\forall y_0 \dots y_{r-1}(\delta\,\varphi)[c_0, \dots, c_{r-1} : y_0, \dots, y_{r-1}] \in \mathrm{T}$ for all $\delta \in \mathrm{T}$ and distinct variables $y_0 \dots y_{r-1}$ not occurring in $\delta\,\varphi$. Assume that $\mathcal{C}$ is a class of structures closed under φ (i. e. $\varphi(U, u_0, \dots, u_{r-1}) \in \mathcal{C}$ for all $U \in \mathcal{C},\ u_0, \dots, u_{r-1} \in \mathrm{dom}(U)$).

Corollary 7.6 $\mathrm{Th}(\mathcal{C})$ *is closed under* φ.

Proof. Suppose $\delta \in \mathrm{Th}(\mathcal{C})$ and $U \in \mathcal{C}$. Then $\varphi(U, u_0, \dots, u_{r-1}) \models \delta$ for all $u_0, \dots, u_{r-1} \in \mathrm{dom}(U)$. By Theorem 7.4 $(U, u_0, \dots, u_{r-1}) \models \delta\,\varphi$ for all $u_0, \dots, u_{r-1} \in \mathrm{dom}(U)$, which implies $U \models \forall y_0 \dots y_{r-1}(\delta\,\varphi)[c_0, \dots, c_{r-1} : y_0, \dots, y_{r-1}] \in \mathrm{T}$ for all distinct variables $y_0 \dots y_{r-1}$ not occurring in $\delta\,\varphi$. $\Diamond$

Corollary 7.7 *Suppose that the theory* T *in* L *is closed under* φ. *Then* $\mathrm{mod}^{\mathrm{L}}(\mathrm{T})$ *is closed under* φ.

Proof. Let $\delta \in \mathrm{T}$, $\gamma = \forall y_0 \dots y_{r-1}(\delta\,\varphi)[c_0, \dots, c_{r-1} : y_0, \dots, y_{r-1}]$ for distinct variables $y_0 \dots y_{r-1}$ not occurring in $\delta\,\varphi$, $U \in \mathrm{mod}^{\mathrm{L}}(\mathrm{T})$ and $u_0, \dots, u_{r-1} \in \mathrm{dom}(U)$. $\gamma \in \mathrm{T}$. Hence $U \models \gamma$. With Theorem 7.4 this implies $\varphi(U, u_0, \dots, u_{r-1}) \models \delta$. Therefore $\varphi(U, u_0, \dots, u_{r-1}) \in \mathrm{mod}^{\mathrm{L}}(\mathrm{T})$. $\Diamond$

Corollary 7.8 $\mathrm{mod}^{\mathrm{L}}(\mathrm{Th}(\mathcal{C}))$ *is closed under* φ. $\Diamond$

Corollary 7.9 *Let* U, V *be structures over* L. *Suppose that* φ *is quantifier bound and that* $U \equiv_{k,r,\mathrm{qr}(\varphi)+m} V$ $(k, m \in \mathbb{N},\ k \geq 1)$. *Then for every* r*-sequence* u *to* $\mathrm{dom}(U)$ *that is connected modulo* k *in* U *there is an* r*-sequence* v *to* $\mathrm{dom}(V)$ *with* $\varphi(U, u), u \equiv_m \varphi(V, v), v$.

Proof. Assume that u is an r-sequence to $\mathrm{dom}(U)$ that is connected modulo k in U. By hypothesis there is an r-sequence v to $\mathrm{dom}(V)$ with $U, u \equiv_{\mathrm{qr}(\varphi)+m} V, v$. This implies $U, u, u \equiv_{\mathrm{qr}(\varphi)+m} V, v, v$. Let δ be a sentence in L_r with $\mathrm{qr}(\delta) = m$. Then $\mathrm{qr}(\delta\varphi) \leq \mathrm{qr}(\varphi) + m$. By setting $t = 2r$ in Theorem 7.4 we have $\varphi(U, u), u \models \delta$ iff $\varphi(U, u, u) \models \delta$ iff $U, u, u \models \delta\varphi$ iff $V, v, v \models \delta\varphi$ iff $\varphi(V, v, v) \models \delta$ iff $\varphi(V, v), v \models \delta$. $\diamondsuit$

Let φ, ψ be interpretations for L of range r, s respectively.

ψ, φ are said to be *composable* iff ψ_R, φ are composable for all $R \in \mathrm{L}$. We define the *composition* $\psi\,\varphi$ of ψ, φ to be the interpretation for L of range $r + s$ with

$$(\psi\,\varphi)_R \;=\; \psi_{\mathbf{R}}\,\varphi$$

for all $R \in \mathrm{L}$. Assume that ψ, φ are composable.

Corollary 7.10 *Let U be a structure over L_t $(t \geq r + s)$.*

$$(\psi\,\varphi)(U) = \psi(\varphi(U)).$$

Proof. For all $R \in \mathrm{L}$ and all ν_R-sequences u to $\mathrm{dom}(U)$

$$\begin{array}{lll} R^{(\psi\,\varphi(U))}(u_0, \ldots, u_{\nu_R - 1}) & \text{iff} & U \models (\psi\,\varphi)_R[u] \quad \text{iff} \\ U \models \psi_R\,\varphi[u] & \text{iff [by Theorem 7.4]} & \varphi(U) \models \psi_R[u] \quad \text{iff} \\ R^{\psi(\varphi(U))}(u_0, \ldots, u_{\nu_R - 1}). & & \end{array}$$ $\diamondsuit$

Corollary 7.11 *Let $\delta(x_0, \ldots, x_{m-1})$ be a formula in L_q $(m, q \in \mathbb{N})$, δ, $\psi\,\varphi$ be composable, U be a structure over L_t $(t \geq q + r + s)$ and u an m-sequence to $\mathrm{dom}(U)$. Then*

$$U \models \delta(\psi\,\varphi)[u] \text{ iff } U \models (\delta\,\psi)\,\varphi[u].$$

By induction the following proposition can be easily verified.

Proposition 7.17 (a) *For all $n \in \mathbb{N}$ the interpretation φ^n for* L *is of range nr and, if φ is quantifier-free, so is φ^n.*

(b) *If φ is quantifier bound,* $\mathrm{qr}(\varphi^n) \leq n\,\mathrm{qr}(\varphi)$ *for all $n \in \mathbb{N}$.*

(c) *Let U, V be structures over* L*. V is φ-derivable in n steps from U iff φ^n defines V in U ($n \in \mathbb{N}$).* $\diamondsuit$

Let $\mathcal{C}$ be a class of structures over L and φ an interpretation for L. We define the *rank with respect* to $\mathcal{C}, \varphi$ of a structure U over L to be the least $i \in \mathbb{N}$ such that φ^i defines U in a structure in $\mathcal{C}$ (i. e. $U \in \varphi^i(\mathcal{C})$), if $U \in \vec{\varphi}(\mathcal{C})$; to be ∞, otherwise. The *rank* of $\mathcal{C}, \varphi$ (*in the finite*) is the highest rank with respect to $\mathcal{C}, \varphi$ of a (finite) structure in $\vec{\varphi}(\mathcal{C})$, if there is the highest rank; it is -1, if $\mathcal{C} = \emptyset$ ($\mathcal{C}^{\mathrm{f}} = \emptyset$); it is ∞, otherwise. Obviously, if the rank of $\mathcal{C}, \varphi$ is in $\mathbb{N}$, then it is the smallest $i \in \mathbb{N}$ with $\vec{\varphi}(\mathcal{C}) = \varphi^{\leq i}(\mathcal{C})$.

Let Σ be a set of sentences in L. $i \in \mathbb{N}$ is a Σ-*bound* of $\mathcal{C}, \varphi$ (*in the finite*) iff every sentence in Σ that is φ-derivable from some (finite) $U \in \mathcal{C}$ is φ-derivable in $\leq i$ steps from some (finite) $U \in \mathcal{C}$. An *elementary bound* of $\mathcal{C}, \varphi$ (*in the finite*) is a Σ-bound of $\mathcal{C}, \varphi$ (in the finite) for the set Σ of all sentences in L. We call the rank respectively an elementary bound of $\mathrm{mod}^{\mathrm{L}}(\theta), \varphi$ (θ a sentence or a theory in L) (in the finite) more simply the *rank* respectively an *elementary bound* of θ, φ (*in the finite*).

Assume that L is finite, φ is a quantifier-free interpretation for L of range 0 and $\mathcal{C}$ a class of structures over L.

For any $n \in \mathbb{N}$ there are only finitely many (logically) inequivalent quantifier-free formulas $\zeta(x_0, \ldots, x_{n-1})$ in L. Therefore there are only finitely many, say k, quantifier-free interpretations for L of range 0. By Proposition 7.17 (a) φ^j is a quantifier-free interpretation for L of range 0 for all $j \in \mathbb{N}$, whence there is $j < k$ with $\varphi^k = \varphi^j$, which implies that for all $i \in \mathbb{N}$ there is $j < k$ with $\varphi^i = \varphi^j$. Therefore, if $U \in \vec{\varphi}(\mathcal{C})$, by Proposition 7.17 (c), $U = \varphi^j(V)$ for some $V \in \mathcal{C}$ and $j < k$, yielding that the rank of U with respect to $\mathcal{C}, \varphi$ is $< k$. We obtain that, if $\mathcal{C} \neq \emptyset$, the rank of $\mathcal{C}, \varphi$ is in $\mathbb{N}$. (If $\mathcal{C} = \emptyset$, the rank is not ∞ either.) With these considerations we can state as a corollary of Proposition 7.17:

Corollary 7.13 *The rank of $\mathcal{C}, \varphi$ is not ∞.* $\diamondsuit$

Corollary 7.13 delivers a notable set of interpretations φ for L for which the rank of $\mathcal{C}, \varphi$ is not ∞, for any class $\mathcal{C}$ of structures over L, namely the set of quantifier-free interpretations for L of range 0. Using this result we obtain, with Corollary 7.14, a large variety of non-trivial classes of structures which are preserved under chains.

Proposition 7.18 *Suppose that $\mathcal{C}$ is preserved under chains. $\vec{\varphi}(\mathcal{C})$ is preserved under chains.*

Proof. First prove that if ψ is a quantifier-free interpretation for L of range r and $(U_\gamma)_{\gamma<\alpha}$ a chain of structures with each U_γ over L_r, then $\psi(\bigcup(U_\gamma)_{\gamma<\alpha}) = \bigcup(\psi(U_\gamma))_{\gamma<\alpha}$. Therefore, for all $i \in \mathbb{N}$, since φ^i is quantifier-free of range 0, $\varphi^i(\mathcal{C})$ is preserved under chains. Because if $\mathcal{D}_0, \ldots, \mathcal{D}_k$ are preserved under chains, so is $\mathcal{D}_0 \cup \ldots \cup \mathcal{D}_k$, for all

$i \in \mathbb{N}$ the class $\varphi^{\leq i}(\mathcal{C})$ is preserved under chains. By Corollary 7.13 $\vec{\varphi}(\mathcal{C}) = \varphi^{\leq i}(\mathcal{C})$ for some $i \in \mathbb{N}$. $\diamondsuit$

Corollary 7.14 *Let $\mathcal{U}$ be a finite set of finite, connected structures over* L. $\vec{\varphi}(\mathrm{cmb}(\mathcal{U}))$ *is preserved under chains.*

Proof. $\mathrm{cmb}(\mathcal{U})$ is axiomatized by a sentence in Π_2^{L}, whence preserved under chains. Now use Proposition 7.18. $\diamondsuit$

We now provide an example of the use of Corollary 7.14. For simplicity, in this example, we write R instead of R_1. If U is a structure over the set S_1 of multigraph symbols, we denote by $\tilde{U}$, $\hat{U}$ and $\neg U$ the structures over S_1 with domain $\mathrm{dom}(U)$ satisfying:

$R^{\tilde{U}}(u, v)$ iff $R^U(u, v)$ for all $u \neq v$ in $\mathrm{dom}(U)$;

$R^{\tilde{U}}(u, u)$ iff not $R^U(u, u)$ for all $u \in \mathrm{dom}(U)$;

not $R^{\hat{U}}(u, v)$ for all $u \neq v$ in $\mathrm{dom}(U)$;

$R^{\hat{U}}(u, u)$ iff not $R^U(u, u)$ for all $u \in \mathrm{dom}(U)$;

$R^{\neg U}(u, v)$ iff not $R^U(u, v)$ for all $u, v \in \mathrm{dom}(U)$.

Let $\mathcal{U}$ be the set of all structures over S_1 with domain $\{0\}$ or $\{0, 1\}$. Set

$\mathcal{A} = \{U \in \mathcal{U} \mid \mathrm{dom}(U) = \{0, 1\}, R^U(0, 0) \text{ and } R^U(1, 1)\}$

and $A, B \in \mathcal{U}$ with domain $\{0, 1\}$ through

$R^A(1, 0)$, not $R^A(0, 1)$, $R^A(0, 0)$ and not $R^A(1, 1)$; $B = \neg A$.

Let $F\colon \mathcal{U} \to \mathcal{U}$ map every $U \in \mathcal{U} \setminus (\mathcal{A} \cup \{A, B\})$ to $\neg U$, every $U \in \mathcal{A}$ to $\tilde{U}$ and $U = A, B$ to $\hat{U}$. F is monotonic. Φ^F is a quantifier-free interpretation for S_1 of range 0. Since,

7.2 φ-derivability in a fixed number of steps from combinations

The proof of Theorem 7.5, which is part of this section, requires the simple combinatorial result expressed in Proposition 7.20. Let $n \in \mathbb{N}$. We call $m_0, \ldots, m_{k-1}$ $(k \geq 1)$ a *factorization* of n iff $m_0 + \ldots + m_{k-1} = n$ and $m_0 \geq m_1 \geq \ldots \geq m_{k-1} > 0$. For $m \in \mathbb{N}$, $m \neq 0$ we define n/m as the largest $k \in \mathbb{N}$ with $k\,m \leq n$. This is also the largest natural number $k \leq \frac{n}{m}$, where $\frac{n}{m}$ denotes the rational quotient of n and m. An i-sequence a to $\mathbb{N}$ *majorizes* a j-sequence b to $\mathbb{N}$ $(i, j \in \mathbb{N})$ iff $j \leq i$ and $b_k \leq a_k$ for all $0 \leq k < j$.

Proposition 7.20 *Suppose $n \neq 0$. $n/1, \ldots, n/n$ majorizes every factorization of n.*

Proof. Let $m_0, \ldots, m_{k-1}$ $(k \geq 1)$ be a factorization of n. Certainly $k \leq n$, since $m_0, \ldots, m_{k-1} \neq 0$. Assume, towards a contradiction, that $m_i > n/(i+1)$ for some $0 \leq i < k$. Then $i \geq 1$ and $m_i > \frac{n}{i+1}$. Hence $m_0 + \ldots + m_{i-1} < \frac{i\,n}{i+1}$. Therefore $m_j < \frac{n}{i+1}$ for a $0 \leq j < i$, which implies $m_j \leq n/(i+1)$, yielding $m_j < m_i$. This contradicts that $m_0, \ldots, m_{k-1}$ is a factorization of n. ◊

Let L be a finite set of relation symbols.

Proposition 7.21 *Let $i \in \mathbb{N}$, $U_0, \ldots, U_i$ and $V_0, \ldots, V_i$ be each an $i+1$-sequence of structures over* L *with disjoint domains and u_j respectively v_j $(0 \leq j \leq i)$ be finite sequences of the same length to* $\mathrm{dom}(U_j)$ *respectively* $\mathrm{dom}(V_j)$*. Assume $U_j, u_j \equiv_m V_j, v_j$ $(0 \leq j \leq i)$. Then $U_0 \oplus \ldots \oplus U_i, (u_0, \ldots, u_i) \equiv_m V_0 \oplus \ldots \oplus V_i, (v_0, \ldots, v_i)$.*

Proof. Immediate consequence of Ehrenfeucht's Theorem. ◊

Let $k, n, m \in \mathbb{N},\ k \geq 1,\ r = nk$. Let furthermore Q be the $(n+m)$-sequence

$$\equiv_{k,(n/1)\cdot k,m}, \ldots, \equiv_{k,(n/n)\cdot k,m}, \equiv_m, \ldots, \equiv_1$$

(notice that $\equiv_m = \equiv_{k,0,m}, \ldots, \equiv_1 = \equiv_{k,0,1}$) and $\mathcal{U}, \mathcal{V} \neq \emptyset$ be sets of structures over L with pairwise disjoint domains.

Theorem 7.5 *Suppose that $\mathcal{A}, \mathcal{B}$ are full Q-choices of $\mathcal{U}, \mathcal{V}$ respectively and $\mathcal{A}_i, \mathcal{B}_i$ are Q_i-equivalent for all $0 \leq i < n+m$. Then $\sum \mathcal{U} \equiv_{k,r,m} \sum \mathcal{V}$.*

Proof. To begin we need some designations. Let $\mathcal{Y} \neq \emptyset$ be a set of structures over L with pairwise disjoint domains. For $y \in \mathrm{dom}(\sum \mathcal{Y})$ we write $[y]_{\mathcal{Y}}$ for the structure $Y \in \mathcal{Y}$ with $y \in \mathrm{dom}(Y)$. Let y be an r-sequence to $\mathrm{dom}(\sum \mathcal{Y})$ that is *completely connected modulo* k in $\sum \mathcal{Y}$, i. e. with the property that for all $0 \leq i < n$ the restriction $\sum \mathcal{Y} | \{u_{ik}, \ldots, u_{(i+1)k-1}\}$ is connected. We define the equivalence relation $\sim^k_{y,\mathcal{Y}}$ over $\{0, \ldots, n-1\}$ by

$i \sim^k_{y,\mathcal{Y}} j$ iff $[y_{ik}]_{\mathcal{Y}} = [y_{jk}]_{\mathcal{Y}}$

for all $0 \leq i, j < n$. For $I \in \{0, \ldots, n-1\} / \sim^k_{y,\mathcal{Y}}$ set $[I]^k_{y,\mathcal{Y}}$ equal $[y_{ik}]_{\mathcal{Y}}$ for some (and whence all) $i \in I$. A bijective i-sequence I to $\{0, \ldots, n-1\} / \sim^k_{y,\mathcal{Y}}$ such that $|I_j| \geq |I_l|$ for all $0 \leq j \leq l < i$ is called an *ordered $y, \mathcal{Y}$-partition modulo k*. Finally for $0 \leq i_0 < \ldots < i_{j-1} < n$ and $I = \{i_0, \ldots, i_{j-1}\}$ set $y^{I,k} = y_{i_0 k}, \ldots, y_{(i_0+1)k}, \ldots, y_{i_{j-1}k}, \ldots, y_{(i_{j-1}+1)k}$.

Now we proceed with the proof. Choose an r-sequence u to $\mathrm{dom}(\sum \mathcal{U})$ that is connected modulo k in $\mathcal{U}$ (for u to $\mathrm{dom}(\sum \mathcal{V})$ the proof proceeds in the symmetrically corresponding way). By eliminating repeated elements in u we can assume that u

$(in+m)_{U\in\mathcal{U}}$ and

$$Q = \equiv_{k,((in)/1)\cdot k,m}, \ldots, \equiv_{k,((in)/(in))\cdot k,m}, \equiv_m, \ldots, \equiv_1 .$$

Theorem 7.7 *Assume that $\bar{U}$ is φ-derivable in $\le i$ steps from a combination U of $\mathcal{U}$. Then there is $\bar{V} \equiv_l \bar{U}$ that is φ-derivable in $\le i$ steps from a combination of $\mathcal{C}$ with coefficients $\le \alpha$.*

Proof. By Proposition 7.17 (a), (c) $\bar{U} = \varphi^j(U,u)$ for some $j \le i$ and some jr-sequence u to $\mathrm{dom}(U)$. Let R be the $jn+m$-sequence

$$\equiv_{k,((jn)/1)\cdot k,m}, \ldots, \equiv_{k,((jn)/(jn))\cdot k,m}, \equiv_m, \ldots, \equiv_1 .$$

R is a $[k,jr,m]$-sequence over $\mathcal{U}$ and E_{j_0} is finer than R_{j_0} for all $0 \le j_0 < jn+m$. Let $\mathcal{U}'' \subseteq \mathcal{U}'$ be a combination set of $\mathcal{U}$ with coefficients $(jn+m)_{U\in\mathcal{U}}$ and $\mathcal{D}$ be a choice set of $\mathcal{U}/R_0$. By Corollary 1.6 $\mathcal{V}$ includes an R-contraction $\mathcal{W}$ of $\mathcal{U}'$. Because, by Proposition 1.2 (d), $\alpha^{\mathcal{W}}_{R_0,\mathcal{U}}(U) \le jn+m$ for all $U \in \mathcal{U}$, there is an injective $F\colon \mathcal{W} \to \mathcal{U}''$ with $R_0(F(W),W)$ for all $W \in \mathcal{W}$. By Proposition 1.2 (a) $F(\mathcal{W}) \subseteq \mathcal{U}''$ is an R-contraction of $\mathcal{U}'$. By Proposition 1.2 (b) $F(W)$ is an R-contraction of $\mathcal{U}''$ and $\alpha^{F(\mathcal{W})}_{R_0,\mathcal{U}} = \alpha^{\mathcal{W}}_{R_0,\mathcal{U}}$. By Corollary 7.20 there is a combination W of $\mathcal{D}$ with coefficients $\le \alpha^{\mathcal{W}}_{R_0,\mathcal{U}}$ satisfying $W \equiv_{k,jr,m} U$. By Corollary 7.19 there is a combination V of $\mathcal{C}$ with coefficients $\le \alpha^{\mathcal{V}}_{E_0,\mathcal{U}} = \alpha$ satisfying $V \equiv_{k,jr,m} W$. We obtain $V \equiv_{k,jr,m} U$. By Proposition 7.19 there are $j_0 \le j \le i$ and a j_0r-sequence v to $\mathrm{dom}(V)$ with $\varphi^{j_0}(V,v) \equiv_l \bar{U}$. $\diamondsuit$

Theorem 7.7 delivers an upper bound for the size of a combination of $\mathcal{U}$ from which some structure of an l-equivalence type is φ-derivable in $\le i$ steps, if a structure of that type is φ-derivable in $\leq i$ steps from a combination of $\mathcal{U}$. (Here by the size of a combination U of $\mathcal{U}$ we mean the smallest cardinality of a combination set of $\mathcal{U}$ whose sum is U.) If the theorem is reformulated with $(in + m)_{U \in \mathcal{U}}$ instead of α, the proof could be carried out by means of Corollary 7.18, instead of Corollary 7.20, which guarantees the existence of a combination V of $\mathcal{C}$ with coefficients $\leq (in+m)_{U \in \mathcal{U}}$ satisfying $V \equiv_{k,ir,m} U$. Since Corollary 7.18, as noted immediately after it, has a direct proof from Ehrenfeucht's Theorem, its use would make the proof of the reformulated version far more straightforward. On the other hand $\alpha \leq (in+m)_{U \in \mathcal{U}}$. If $\mathcal{U}$ is a finite set of finite structures over L, both Theorem 7.7 and its reformulated version lead to a procedure that solves the problem whether a sentence in L is φ-derivable in $\leq i$ steps from a combination of $\mathcal{U}$. Whether Theorem 7.7 leads to a relevantly lower complexity of the problem will not be examined in this book and remains therefore an open question. In any case, it delivers strikingly lower upper bounds in the examples that will follow in the next section.

Corollary 7.21 *Every sentence that is φ-derivable in $\leq i$ steps from a combination of $\mathcal{U}$ is already φ-derivable in $\leq i$ steps from a finite-combination of $\mathcal{U}$.* $\diamondsuit$

Let $\mathcal{U}$ be a set of finite structures over L.

The next corollary is a rather expected and yet not obvious consequence of Theorem 7.7.

Corollary 7.22 *Assume that to* L *belongs a non-monadic relation symbol. Then there is no interpretation* ψ *for* L *such that* $\vec{\psi}(\mathrm{cmb}(\mathcal{U}))$ *is the class of all structures over* L.

Proof. Towards a contradiction let ψ be an interpretation for L of range r such that $\vec{\psi}(\mathrm{cmb}(\mathcal{U}))$ is the class of all structures over L and δ be an axiom of infinity in L. Then δ is ψ-derivable from a combination of $\mathcal{U}$, whence, by Corollary 7.21, from a finite-combination of $\mathcal{U}$, which is a finite structure over L. But this is not possible, being δ an axiom of infinity. $\diamondsuit$

Corollary 7.23 $i \in \mathbb{N}$ *is an elementary bound of* $\mathrm{cmb}(\mathcal{U}), \varphi$ *iff* i *is an elementary bound of* $\mathrm{cmb}(\mathcal{U}), \varphi$ *in the finite.*

Proof. $\Rightarrow$. Assume i is an elementary bound of $\mathrm{cmb}(\mathcal{U}), \varphi$ and that δ is a sentence in L which is φ-derivable from a finite combination of $\mathcal{U}$. Then δ is φ-derivable in $\leq i$ steps from some combination of $\mathcal{U}$. By Corollary 7.21 δ is φ-derivable in $\leq i$ steps from a finite combination of $\mathcal{U}$. $\Leftarrow$. Now assume that i is an elementary bound of $\mathrm{cmb}(\mathcal{U}), \varphi$ in the finite and that δ is a sentence in L which is φ-derivable from a combination of $\mathcal{U}$. By Corollary 7.21 δ is φ-derivable from a finite combination of $\mathcal{U}$, whence in $\leq i$ steps from a finite combination of $\mathcal{U}$. $\diamondsuit$

Corollary 7.24 $\mathrm{Th}((\vec{\varphi}(\mathrm{cmb}(\mathcal{U})))^{\mathrm{f}}) = \mathrm{Th}(\vec{\varphi}(\mathrm{cmb}(\mathcal{U})))$. $\diamondsuit$

Corollary 7.25 *If* $\mathcal{U}$ *is finite and the rank of* $\mathrm{cmb}(\mathcal{U}), \varphi$ *is not* ∞*, then the* φ*-derivability problem for* $\mathrm{cmb}(\mathcal{U})$ *is solvable.* $\diamondsuit$

Proposition 7.25 *Assume that $\bar{U}$ is φ-derivable in $\leq i$ steps from a combination of $\mathcal{U}$. Then there is $\bar{V} \equiv_l \bar{U}$ that is φ-derivable in $\leq i$ steps from a combination of $\mathcal{U}$ with coefficients $\leq (in+m)_{U\in\mathcal{U}}$.*

Proof. Let $\mathcal{V}$ be a combination set of $\mathcal{U}$ and assume that $\bar{U}$ is φ-derivable in $\leq i$ steps from $\sum\mathcal{V}$. By Proposition 7.17 (a), (c) there is a jr-sequence v to $\mathrm{dom}(\sum\mathcal{V})$ with $\varphi^j(\sum\mathcal{V}, v) = \bar{U}$ ($j \leq i$). Let $\mathcal{W} \subseteq \mathcal{V}$ satisfy the condition that for every $V \in \mathcal{V}$ there are as many structures in $\mathcal{W}$ isomorphic to V as there are in $\mathcal{V}$ or exactly $jn+m$ structures in $\mathcal{W}$ isomorphic to V. Obviously $\sum\mathcal{W}$ is a combination of $\mathcal{U}$ with coefficients $\leq (in+m)_{U\in\mathcal{U}}$. By the comment immediately following Corollary 7.18, stating that this corollary with "k, r, m-equivalent" replaced by "isomorphic" still holds for sets $\mathcal{U}, \mathcal{V} \neq \emptyset$ of structures with pairwise disjoint domains over an infinite set of symbols, $\sum\mathcal{V} \equiv_{k,jr,m} \sum\mathcal{W}$. By Proposition 7.19 there are $j_0 \leq j \leq i$ and a j_0r-sequence w to $\mathrm{dom}(\sum\mathcal{W})$ with $\varphi^{j_0}(\sum\mathcal{W}, w) \equiv_l \bar{U}$, whence $\bar{U}$ is φ-derivable in j_0 steps from $\sum\mathcal{W}$. ♢

Corollary 7.27 *Corollary* 7.21 *still holds, if $\mathcal{U}$ is finite.* ♢

7.3 Application of Theorem 7.7 to k- and $\langle l,k\rangle$-paths

As an illustration of the use of Theorem 7.7, we apply it to k- and $\langle l,k\rangle$-paths. These examples will show how Theorem 7.7 allows to obtain decent upper bounds for the size of a sufficient combination. The meaning of n/m has been given in Section 7.2.

Let $r, m, i, n \in \mathbb{N}$, $m \geq 2$, $i, n \neq 0$, $r = n2$ and

$$Q = \equiv_{2,((in)/1)\cdot 2,m}, \ldots, \equiv_{2,((in)/(in))\cdot 2,m}, \equiv_m, \ldots, \equiv_1 .$$

We define h_j and $\bar{h}_j$ ($1 \leq j \leq in + m$) through

$$\begin{array}{lcll} h_j & = & 2^m((in)/j+1) + 2((in)/j) - 1, & \text{if } 1 \leq j \leq in; \\ h_{in+j} & = & 2^{m-j+1}, & \text{if } 1 \leq j < m; \\ h_{in+m} & = & 1; & \\ \bar{h}_j & & \text{is the smallest even number } \geq h_j + (in)/j - 1, & \text{if } 1 \leq j \leq in; \\ \bar{h}_{in+j} & = & h_{in+j}, & \text{if } 1 \leq j < m; \\ \bar{h}_{in+m} & = & 2. & \end{array}$$

We begin with the application to k-paths. Let U_k ($k \in \mathbb{N}$) be the k-path with domain $\{0, \ldots, k+1\}$, $P^{U_k}(0)$ and $R_1^{U_k}(i,j)$ iff $j = i+1$ ($0 \leq i \leq j \leq k+1$). We set $\mathcal{U}_k = \{U_j \,|\, 0 \leq j \leq k\}$ and $\mathcal{K} = \{U_k \,|\, k \in \mathbb{N}\}$. Obviously the class of all structures that are k- paths for some $k \in \mathbb{N}$ is the class of all structures isomorphic to a structure in $\mathcal{K}$.

We now introduce a Q-combination function α over $\mathcal{K}$ by setting:

$$\begin{aligned} \alpha(U_k) &= 1, && \text{if } h_2 \leq k; \\ \alpha(U_k) &= j, && \text{if } h_{j+1} \leq k < h_j \text{ and } 2 \leq j < in+m; \\ \alpha(U_0) &= in+m. \end{aligned} \tag{1}$$

Given that, by Theorem 6.3, $\mathcal{U}_{h_j}$ is a choice set of $\mathcal{K}/Q_{j-1}$ and that

$$h_1 - h_j + 2 > 2j, \tag{2}$$

whence $h_1 - h_j + 1 > j$, for all $2 \leq j \leq in+m$, we obtain that α is really a Q-combination function over $\mathcal{K}$. We have that

$$|\mathcal{K}|_Q = 1 + \sum_{j=1}^{in+m} h_j = (2^m+2)\sum_{j=1}^{in}(in)/j \ + 2^m(in+2) - in - 2.$$

Assume that φ is a modulo 2 connected interpretation for $\{P, Q, R_1\}$ of range r and $m = i\mathrm{qr}(\varphi) + m_0$ ($m_0 \in \mathbb{N}$). With Theorem 7.7 we conclude:

Proposition 7.26 *A first-order property expressible in* $\{P, Q, R_1\}$ *with quantifier rank* m_0 *is* φ*-derivable in* $\leq i$ *steps from a combination of* $\mathcal{K}$ *iff it is* φ*-derivable in* $\leq i$ *steps from a combination of* $\mathcal{U}_{h_1}$ *with coefficients* $\leq \alpha$ *and therefore from an at most* $|\mathcal{K}|_Q$*-combination of* $\mathcal{U}_{h_1}$*.* $\diamondsuit$

We now turn to the application of Theorem 7.7 to $\langle l,k\rangle$-paths. Let $U_{l,k}$ ($l, k \in \mathbb{N}$) be the $\langle l,k\rangle$-path with domain $\{0,\ldots,l+k+2\}$, $P^{U_{l,k}}(0)$ and for all $0 \leq i \leq j \leq l+k+1$

$R_1^{U_{l,k}}(i,j)$ iff $j = i+1$ and one of the two conditions $i > l$ or i even holds,

$R_2^{U_{l,k}}(i,j)$ iff $j = i+1$, $i \leq l$ and i odd.

Assume that φ is a modulo 2 connected interpretation for $\{P, Q, S, R_1, R_2\}$ of range r and $m = i\mathrm{qr}(\varphi) + m_0$ ($m_0 \in \mathbb{N}$). With Theorem 7.7 we conclude:

Proposition 7.27 *A first-order property expressible in* $\{P, Q, S, R_1, R_2\}$ *with quantifier rank* m_0 *is* φ*-derivable in* $\leq i$ *steps from a combination of* $\mathcal{L}$ *iff it is* φ*-derivable in* $\leq i$ *steps from a combination of* $\mathcal{U}_{\bar{h}_1,h_1}$ *with coefficients* $\leq \alpha$ *and therefore from an at most* M*-combination of* $\mathcal{U}_{\bar{h}_1,h_1}$. ♢

To give a numerical example of Proposition 7.26, set $r = 4$, which implies $n = 2$, $m = 6$, $i = 4$ and $\mathrm{qr}(\varphi) = 1$.

$((in)/j)_{1\leq j\leq in} = (8/j)_{1\leq j\leq 8} = 8, 4, 2, 2, 1, 1, 1, 1,$

$Q = \equiv_{2,(8/1)\cdot 2,6}, \ldots, \equiv_{2,(8/8)\cdot 2,6}, \equiv_6, \ldots, \equiv_1,$

$(h_j)_{1\leq j\leq 14} = 591, 327, 195, 195, 129, 129, 129, 129, 64, 32, 16, 8, 4, 1,$

$|\mathcal{U}|_Q = 1950.$

Hence, with α as in (1), a first-order property expressible in $\{P, Q, R_1\}$ with quantifier rank 2 is φ-derivable in 4 steps from a combination of $\mathcal{K}$ iff it is φ-derivable in 4 steps from a combination of $\mathcal{U}_{591}$ with coefficients $\leq \alpha$, whence from an at most 1950-combination of $\mathcal{U}_{591}$.

Now let's give a numerical example of Proposition 7.27. We set $r = 4$, which implies $n = 2$, $m = 5$, $i = 3$ and $\mathrm{qr}(\varphi) = 1$.

$((in)/j)_{1\leq j\leq in} = (6/j)_{1\leq j\leq 6} = 6, 3, 2, 1, 1, 1,$

$Q = \equiv_{2,(6/1)\cdot 2,5}, \ldots, \equiv_{2,(6/6)\cdot 2,5}, \equiv_5, \ldots, \equiv_1,$

$(h_j)_{1\leq j\leq 11} = 235, 133, 99, 65, 65, 65, 32, 16, 8, 4, 1,$

$(\bar{h}_j)_{1\leq j\leq 11} = 240, 136, 100, 66, 66, 66, 32, 16, 8, 4, 2,$

$M = 49666.$

Hence, with α as in (3), a first-order property expressible in $\{P, Q, S, R_1, R_2\}$ with quantifier rank 2 is φ-derivable in 3 steps from a combination of $\mathcal{L}$ iff it is φ-derivable in 3 steps from a combination of $\mathcal{U}_{240,235}$ with coefficients $\leq \alpha$, whence from an at most 49666-combination of $\mathcal{U}_{240,235}$.

On one hand, as we announced at the beginning of this section, the upper bounds 591 and 1950 respectively (240, 235) and 49666, are of decent size. On the other hand, they may indicate, against an intuitional approach, that first-order properties of quantifier rank 2 could be φ-derivable in 4 respectively 3 steps from $\mathcal{K}$ respectively $\mathcal{L}$, without being φ-derivable from very small combinations.

As a third example, let $\mathcal{U} = \{U_{36,52}, U_{36,51}, U_{34,52}, U_{34,51}, U_{16,51}, U_{16,52}, U_{16,53}, U_{16,54}\}$ and $Q = \equiv_{2,8,4}, \equiv_{2,4,4}, \equiv_{2,2,4}, \equiv_{2,2,4}, \equiv_4, \equiv_3, \equiv_2, \equiv_1$. As we did in the two previous examples, in order to apply Theorem 7.7 to $\mathcal{U}$, we aim at constructing a Q-combination function over $\mathcal{U}$. For this purpose we first build a Q-contraction of a combination set $\mathcal{U}'$ of $\mathcal{U}$ with coefficients $(8)_{U\in\mathcal{U}}$. A Q-contraction is obtained from a full Q-choice $\mathcal{C}$ of $\mathcal{U}'$. Because of Proposition 6.26 $\mathcal{U}$ is a choice set of $\mathcal{U}/Q_0$, whence we can set $\mathcal{C}_0$ to be a combination set of $\mathcal{U}$ with coefficients $(1)_{U\in\mathcal{U}}$. Because of Proposition 6.26 and Proposition 6.22 we have

$\mathcal{U}/Q_1 = \{\{U_{36,52}, U_{36,51}\}, \{U_{34,52}, U_{34,51}\}, \{U_{16,51}, U_{16,52}, U_{16,53}, U_{16,54}\}\},$

whence $\mathcal{C}_1 = \emptyset$;

$\mathcal{U}/Q_2 = \{\{U_{36,52}, U_{36,51}, U_{34,52}, U_{34,51}\}, \{U_{16,51}, U_{16,52}, U_{16,53}, U_{16,54}\}\}$, whence $\mathcal{C}_2 = \emptyset$;

$\mathcal{U}/Q_3 = \mathcal{U}/Q_2$, whence $\mathcal{C}_3 = \emptyset$.

Finally, by Proposition 6.22, $\mathcal{C}_4 = \{\mathcal{U}\}$, whence $\mathcal{C}_4 = \mathcal{C}_5 = \mathcal{C}_6 = \mathcal{C}_7 = \emptyset$. Therefore $\mathcal{C}_0$ is a Q-contraction of $\mathcal{U}'$ and $(1)_{U\in\mathcal{U}}$ a Q-combination function over $\mathcal{U}$.

Let φ be a modulo 2 connected interpretation for $\{P, Q, S, R_1, R_2\}$ of range 4 with $\mathrm{qr}(\varphi) = 1$. Theorem 7.7 implies that a first-order property expressible in $\{P, Q, S, R_1, R_2\}$ with quantifier rank 2 is φ-derivable in ≤ 2 steps from a combination of $\mathcal{U}$ iff it is φ-derivable in ≤ 2 steps from a combination of $\mathcal{U}$ with coefficients $\leq (1)_{U\in\mathcal{U}}$.

In the case that α is a combination function over $\mathcal{U}$ with $\alpha(V) \neq 0$ for all $V \in \mathcal{U}$ and $\mathcal{V}$ a combination set of $\mathcal{U}$ with coefficients α, $\mathcal{C}_0$ can be set to be a Q-contraction of $\mathcal{V}$, as our previous construction easily shows. By Corollary 7.15 $\sum \mathcal{C}_0 \equiv_{2,8,4} \sum \mathcal{V}$. With Proposition 7.17 and Proposition 7.19 we obtain that a first-order property expressible in $\{P, Q, S, R_1, R_2\}$ with quantifier rank 2 is φ-derivable in ≤ 2 steps from a combination of $\mathcal{U}$ with coefficients α iff it is φ-derivable in ≤ 2 steps from a combination of $\mathcal{U}$ with coefficients $(1)_{U\in\mathcal{U}}$ (i. e. from $\sum \mathcal{C}_0$).

As a final example we consider the set $\mathcal{V} = \mathcal{U} \cup \{U_{34,34}\}$, where $\mathcal{U}$ is the set in the third example. It is left as an excercise for the reader to show that $\beta \colon \mathcal{V} \to \mathbb{N}$ with

$\beta(U) = 1$, if $U \in \mathcal{U}$; $\beta(U_{34,34}) = 2$

is Q-combination function over $\mathcal{V}$, while $\mathcal{V}$ is a choice set of $\mathcal{V}/Q_0$, where Q is again as in the third example. Theorem 7.7 yields that a first-order property expressible in

$\{P, Q, S, R_1, R_2\}$ with quantifier rank 2 is φ-derivable in ≤ 2 steps from a combination of $\mathcal{V}$ iff it is φ-derivable in ≤ 2 steps from a combination of $\mathcal{V}$ with coefficients $\leq \beta$.

7.4 Weakly invertible interpretations

Till the end of this section let L be a set of relation symbols.

An interpretation φ for L of range r is called *weakly invertible* iff there is an interpretation ψ for L of range r satisfying for all $U \in \mathrm{dom}(\varphi)$

$$(\psi\,\varphi)(U, (c_{r+i} : c_i^U)_{0\leq i<r}) = U \restriction \mathrm{L} \tag{4}$$

and for all $U \in \mathrm{dom}(\psi)$

$$(\varphi\,\psi)(U, (c_{r+i} : c_i^U)_{0\leq i<r}) = U \restriction \mathrm{L}. \tag{5}$$

Alternatively, satisfying for all structures U over L and all r-sequences u to $\mathrm{dom}(U)$

if $(U, u) \in \mathrm{dom}(\varphi)$, $(\psi\,\varphi)(U, u, u) = U$,

if $(U, u) \in \mathrm{dom}(\psi)$, $(\varphi\,\psi)(U, u, u) = U$.

Proposition 7.28 *There is exactly one interpretation ψ for* L *of range r satisfying* (4) *for all $U \in \mathrm{dom}(\varphi)$ and* (5) *for all $U \in \mathrm{dom}(\psi)$, if there is one. This ψ is written φ'.*

Proof. Assume that (4) holds for all $U \in \mathrm{dom}(\varphi)$, (5) holds for all $U \in \mathrm{dom}(\psi)$ and, with $\psi = \phi$, that (4) holds for all $U \in \mathrm{dom}(\varphi)$, (5) holds for all $U \in \mathrm{dom}(\phi)$. First remark that, if $U \in \mathrm{dom}(\phi)$, then $(\phi(U), (c_i^U)_{0\leq i<r}) \in \mathrm{dom}(\varphi)$. Suppose $U \notin \mathrm{dom}(\psi)$.

If $U \in \mathrm{dom}(\phi)$, then

$$\begin{aligned} U\restriction \mathrm{L} &= \psi((\varphi\,\phi)(U,(c_{r+i},c_{2r+i}:c_i^U)_{0\le i<r})) = (\psi\,\varphi)(\phi(U),(c_i^U)_{0\le i<r},(c_{r+i}:c_i^U)_{0\le i<r}) \\ &= \phi(U), \end{aligned}$$

which is a contradiction. Hence $U \notin \mathrm{dom}(\phi)$. This proves $\psi(U) = U\restriction \mathrm{L} = \phi(U)$. Now suppose $U \in \mathrm{dom}(\psi)$. Then, analogously to the previous remark, $(\psi(U),(c_i^U)_{0\le i<r}) \in \mathrm{dom}(\varphi)$. Thus

$$\begin{aligned} \phi(U) = &\quad \phi((\varphi\,\psi)(U,(c_{r+i},c_{2r+i}:c_i^U)_{0\le i<r})) = (\phi\,\varphi)(\psi(U),(c_i^U)_{0\le i<r},(c_{r+i}:c_i^U)_{0\le i<r}) \\ &= \psi(U). \end{aligned}$$ ♢

Proposition 7.29 *Assume that φ is a weakly invertible interpretation for* L *of range r, $U, V \in \mathrm{dom}(\varphi)$ and f an isomorphism from $\varphi(U)$ to $\varphi(V)$ with $f(c_i^U) = c_i^V$ $(0 \le i < r)$. Then f is an isomorphism from U to V.*

Proof. f is an isomorphism from $(\varphi(U),(c_i^U)_{0\le i<r})$ to $(\varphi(V),(c_i^V)_{0\le i<r})$. Hence from $U\restriction \mathrm{L} = \varphi'(\varphi(U),(c_i^U)_{0\le i<r})$ to $V\restriction \mathrm{L} = \varphi'(\varphi(V),(c_i^V)_{0\le i<r})$. Given that $U = U\restriction \mathrm{L},(c_i^U)_{0\le i<r}$ and $V = V\restriction \mathrm{L},(c_i^V)_{0\le i<r}$, we obtain the claim. ♢

Let $r \in \mathbb{N}$ and φ be a weakly invertible interpretation for L of range r.

Proposition 7.30 *Let γ be a sentence in L_r. $\varphi|\gamma$ is weakly invertible and*

$$(\varphi|\gamma)' = \varphi'|(\gamma\,\varphi')[c_r,\dots,c_{2r-1}\colon c_0,\dots,c_{r-1}].$$

Proof. Let $U \in \mathrm{dom}(\varphi|\gamma)$. To simplify the notation we set

$U^+ = (U,(c_{r+i}\colon c_i^U)_{0\le i<r})$, $c = c_0,\dots,c_{r-1}$, $c^+ = c_r,\dots,c_{2r-1}$, $c^{++} = c_{2r},\dots,c_{3r-1}$.

We first want to prove that

$$(\varphi'|(\gamma\,\varphi')[c^+\colon c])(\varphi|\gamma)(U^+) = U\restriction \mathrm{L}.$$

We immediately obtain that $U \models \gamma$, otherwise $(\varphi|\gamma)(U) = U \restriction \mathrm{L}$. This implies $(\varphi|\gamma)(U) = \varphi(U)$. Hence $\varphi(U) \neq U\restriction \mathrm{L}$. The following equivalences hold:

$$\begin{array}{ll}
U \models \gamma & \text{iff} \\
(\varphi'\,\varphi)(U^+, (c_{2r+i}\colon c_i^U)_{0\le i<r}) \models \gamma & \text{iff [Theorem 7.4]} \\
(U^+, (c_{2r+i}\colon c_i^U)_{0\le i<r}) \models \gamma\,(\varphi'\,\varphi) & \text{iff} \\
U^+ \models (\gamma\,(\varphi'\,\varphi))[c^{++}\colon c^+] & \text{iff [Corollary 7.11]} \\
U^+ \models ((\gamma\,\varphi')\,\varphi)[c^{++}\colon c^+] & \text{iff} \\
U^+ \models ((\gamma\,\varphi')[c^+\colon c])\,\varphi & \text{iff [Theorem 7.4]} \\
\varphi(U^+) \models (\gamma\,\varphi')[c^+\colon c]. &
\end{array}$$

With the conclusions just obtained, we can write:

$(\varphi'|(\gamma\,\varphi')[c^+\colon c])(\varphi|\gamma)(U^+) = (\varphi'|(\gamma\,\varphi')[c^+\colon c])(\varphi(U^+)) = \varphi'(\varphi(U^+)) = U\restriction \mathrm{L}.$

Now let $U \in \mathrm{dom}(\varphi'|(\gamma\,\varphi')[c^+\colon c])$. We show that

$$(\varphi|\gamma)(\varphi'|(\gamma\,\varphi')[c^+\colon c])(U^+) = U\restriction \mathrm{L}.$$

Again, we immediately obtain that $U \models (\gamma\,\varphi')[c^+ : c]$. This implies $(\varphi'|(\gamma\,\varphi')[c^+ : c])(U) = \varphi'(U)$. Hence $\varphi'(U) \neq U\restriction \mathrm{L}$. We have the equivalences:

$$U \models (\gamma\,\varphi')[c^+\colon c] \text{ iff } U^+ \models (\gamma\,\varphi') \text{ iff } \varphi'(U^+) \models \gamma.$$

With these conclusions we can again write:

[5] C. C. Chang, H. J. Keisler, *Model Theory*, 3rd ed., Dover Publications, Inc., Mineola, New York, 2012, pp. 211–223.

[6] W. Hodges, *A shorter model theory*, Cambridge University Press, Cambridge, 1997, pp. 237–249.

[7] K. Potthof, *Einführung in die Modelltheorie und ihre Anwendungen*, Wissenschaftliche Buchgesellschaft, Darmstadt, 1981, pp. 146–154.

8 Preservation theorems

The question that probably condenses in the best way all questions asked in this book is: “What can we state about $\vec{\varphi}(\mathcal{C})$?” given an interpretation φ for L and a class $\mathcal{C}$ of structures over L. For example, as a consequence of Proposition 7.5, if $\mathcal{C}$ is closed under isomorphisms, so is $\vec{\varphi}(\mathcal{C})$. As we will see, for a sentence θ in L, if φ is weakly invertible, $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ is closed under elementary equivalence. On the other hand, it is not necessarily closed under ultraproducts (while $\mathrm{mod}^{\mathrm{L}}(\theta)$, indeed, is).

In this chapter we study certain preservation properties of axiomatizable classes of structures. This study is mainly another presentation of known model theoretical results [1]. If $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ is axiomatizable and φ quantifier-free as well as weaky invertible, these preservation properties of $\mathrm{mod}^{\mathrm{L}}(\theta)$ translate into corresponding preservation properties of $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$.

For structures U, V over a set S of symbols, Σ a set of sentences in S and α a cardinal we write $U \Rightarrow_{\Sigma} V$ iff every sentence in Σ true in U is true in V and call U, for simplicity under the harmless assumption that $\mathrm{dom}(U) \cap \mathrm{S} = \emptyset$, *$\alpha$-saturated* iff for every $A \subseteq \mathrm{dom}(U)$ with $|A| < \alpha$ the expansion (U, A) realizes all sets of formulas $\xi(x_0)$ in $\mathrm{S} \cup A$ consistent with $\mathrm{Th}(U, A)$. Generalizing the definition of m-sequence and of sequence, an *α-sequence* (to the set A or of elements of A) is a function u with $\mathrm{dom}(u) = \alpha$ ($\mathrm{rg}(u) \subseteq A$) in which $u(\gamma)$ is denoted by u_γ for all $\gamma < \alpha$. Given v_γ for all $\gamma < \alpha$, we write $(v_\gamma)_{\gamma<\alpha}$ to designate the α-sequence u with $u_\gamma = v_\gamma$ for all $\gamma < \alpha$.

Let L be a set of symbols, α a cardinal, U, V structures over L and c an injective α-sequence of constants not in L. For $\gamma < \alpha$, a structure W over L and a γ-sequence w to $\mathrm{dom}(W)$ we denote by (W, w) the expansion $(W, (c_\delta\colon w_\delta)_{\delta<\gamma})$.

Proposition 8.1 *Let v be an α-sequence to* $\mathrm{dom}(V)$. *Assume* $U \Rightarrow_{\Pi_i^{\mathrm{L}}} V$ $(1 \leq i \in \mathbb{N})$ *and that U is α-saturated. Then there is an α-sequence u to* $\mathrm{dom}(U)$ *with*

$$(U, u) \Rightarrow_{\Pi_i^{\mathrm{L}\cup\{c_\gamma\,|\,\gamma<\alpha\}}} (V, v).$$

Proof. By transfinite induction over α, we form an increasing (with respect to the restriction property) α-sequence $(u^\gamma)_{\gamma<\alpha}$ of γ-sequences u^γ to $\mathrm{dom}(U)$ satisfying for all $\gamma < \alpha$

$$(U, u^\gamma) \Rightarrow_{\Pi_i^{\mathrm{L}\cup\{c_\delta\,|\,\delta<\gamma\}}} (V, v|\gamma). \tag{1}$$

By hypothesis (1) holds for $\gamma = 0$. If γ is a limit ordinal set $u^\gamma = \bigcup_{\delta<\gamma} u^\delta$. Let $\gamma < \alpha$ and Δ be the set of all sentences in $\Sigma_i^{\mathrm{L}\cup\{c_\delta\,|\,\delta\leq\gamma\}}$ that hold in $(V, v|(\gamma+1))$. $\mathrm{Th}(U, u^\gamma) \cup \Delta$ is consistent. Otherwise there would be a sentence in $\Sigma_i^{\mathrm{L}\cup\{c_\delta\,|\,\delta<\gamma\}}$ true in $(V, v|\gamma)$, but failing in (U, u^γ), which contradicts the induction hypothesis. Since U is α-saturated there is an expansion $(U, u^\gamma, c_\gamma\colon a)$ of (U, u^γ) satisfying Δ. This ends the transfinite induction over α. Now set $u = \bigcup_{\gamma<\alpha} u^\gamma$. $\diamondsuit$

For the next Proposition 8.2 and Proposition 8.3 assume $\mathrm{L} \cap \mathrm{dom}(V) = \emptyset$.

Proposition 8.2 *Suppose* $U \Rightarrow_{\Pi_i^{\mathrm{L}}} V$ $(1 \leq i \in \mathbb{N})$. *Then there is U_0 over* L *with* $\mathrm{dom}(V) \subseteq \mathrm{dom}(U_0)$ *such that U is elementarily embedded into U_0 and*

$$(U_0, \mathrm{dom}(V)) \Rightarrow_{\Pi_i^{\mathrm{L}\cup\mathrm{dom}(V)}} (V, \mathrm{dom}(V)).$$

Proof. Let α be a cardinal with $\alpha \geq |\mathrm{dom}(V)|$. There is an α-saturated U_0 into which U is elementarily embedded [2]. Let v be an α-sequence of elements of $\mathrm{dom}(V)$ surjective to $\mathrm{dom}(V)$ (in other words, an α-sequence which is an enumeration of $\mathrm{dom}(V)$). By Proposition 8.1 there is an α-sequence u to $\mathrm{dom}(U_0)$ with $(U_0, u) \Rightarrow_{\Pi_i^{\mathrm{L}\cup\{c_\gamma \mid \gamma<\alpha\}}} (V, v)$. Indeed, we can assume $u = v$. This means $(U_0, \mathrm{dom}(V)) \Rightarrow_{\Pi_i^{\mathrm{L}\cup\mathrm{dom}(V)}} (V, \mathrm{dom}(V))$ and that U_0 is as in the claim. $\diamondsuit$

Proposition 8.3 *Assume* $\mathrm{dom}(U) \subseteq \mathrm{dom}(V)$ *and* $(U, \mathrm{dom}(U)) \Rightarrow_{\Pi_{i+1}^{\mathrm{L}\cup\mathrm{dom}(U)}} (V, \mathrm{dom}(U))$ $(i \in \mathbb{N})$*. Then there is an elementary extension* U_0 *of* U *with* $\mathrm{dom}(V) \subseteq \mathrm{dom}(U_0)$ *and*

$$(V, \mathrm{dom}(V)) \Rightarrow_{\Pi_i^{\mathrm{L}\cup\mathrm{dom}(V)}} (U_0, \mathrm{dom}(V)).$$

Proof. Let Δ be the set of sentences in $\Pi_i^{\mathrm{L}\cup\mathrm{dom}(V)}$ true in $(V, \mathrm{dom}(V))$. $\mathrm{Th}(U, \mathrm{dom}(U)) \cup \Delta$ is consistent. Otherwise there would be a sentence in $\Sigma_{i+1}^{\mathrm{L}\cup\mathrm{dom}(U)}$ true in $(V, \mathrm{dom}(U))$, but false in $(U, \mathrm{dom}(U))$, contradicting the hypothesis. Therefore there is U_0 as in the thesis. $\diamondsuit$

Proposition 8.4 *Assume* $\mathrm{dom}(U) \subseteq \mathrm{dom}(V)$*. If* $(U, \mathrm{dom}(U)) \Rightarrow_{\Pi_i^{\mathrm{L}\cup\mathrm{dom}(U)}} (V, \mathrm{dom}(U))$ $(1 \leq i \in \mathbb{N})$*, then there are structures* $U_0, \ldots, U_{i-1}$ *over* L *with*

$V \subseteq U_0 \subseteq \ldots \subseteq U_{i-1}$,

$U \preceq U_0$,

$U_j \preceq U_{j+2}$ $(0 \leq j < i-2)$ *and*

$V \preceq U_1$, *if* $i \geq 2$.

Lemma 8.1 *Assume that if $U \models \mathrm{T}$ and $U \Rightarrow_{\Pi_i^{\mathrm{L}}} V$, then $V \models \mathrm{T}$ $(i \in \mathbb{N})$. Then* T *is axiomatized by a set of sentences in Π_i^{L}.*

Proof. Let Δ be the set of all sentences in Π_i^{L} that follow from T. Assume $V \models \Delta$. Let Γ be the set of all sentences in Σ_i^{L} that hold in V. $\mathrm{T} \cup \Gamma$ has a model U. Otherwise there would be a sentence in Δ failing in V, which is a contradiction. $U \models \mathrm{T}$ and $V \Rightarrow_{\Sigma_i^{\mathrm{L}}} U$, whence $U \Rightarrow_{\Pi_i^{\mathrm{L}}} V$. By hypothesis $V \models \mathrm{T}$. $\diamondsuit$

In a completely analogous way the following lemma can be proven:

Lemma 8.2 *Assume that if $U \models \mathrm{T}$ and $U \Rightarrow_{\Sigma_i^{\mathrm{L}}} V$, then $V \models \mathrm{T}$ $(i \in \mathbb{N})$. Then* T *is axiomatized by a set of sentences in Σ_i^{L}.* $\diamondsuit$

Theorem 8.2 *Let $1 \leq i \in \mathbb{N}$ and* T *be a theory in* L. $\mathrm{mod}^{\mathrm{L}}(T)$ *is preserved under i-sandwiches iff* T *is axiomatized by a set of sentences in Π_i^{L}. If* T *is finite and* $\mathrm{mod}^{\mathrm{L}}(T)$ *is preserved under i-sandwiches, then it is axiomatized by a sentence in Π_i^{L}.*

Proof. Assume $\mathrm{mod}^{\mathrm{L}}(T)$ is preserved under i-sandwiches. By Theorem 8.1, if $U \models \mathrm{T}$ and $U \Rightarrow_{\Pi_i^{\mathrm{L}}} V$, then $V \models \mathrm{T}$. With Lemma 8.1 T is axiomatized by a set of sentences in Π_i^{L}. The other direction is obvious, given Theorem 8.1. By Compactness, if T is finite, it follows already from a finite set of sentences in Π_i^{L}. $\diamondsuit$

Using Corollary 8.1 instead of Theorem 8.1 and Lemma 8.2 instead of Lemma 8.1 we obtain:

$$\text{dom}(U) = \{0,1\} \text{ and } (U,\{0,1\}) \models (\ (\neg R\,0\,0 \leftrightarrow R\,1\,1) \wedge$$
$$(R\,0\,1 \leftrightarrow R\,1\,0)\ )\}.$$

Let $F\colon \mathcal{U} \to \mathcal{U}$ map A to $\tilde{A}$, C to $\tilde{C}$, every $U \in \mathcal{A} \cup \{B, D\}$ to $\neg U$ and every $U \in \mathcal{U} \setminus (\mathcal{A} \cup \{A, B, C, D\})$ to U. F is monotonic and injective. Its inverse F^{-1} is also monotonic. By Proposition 7.35 Φ^F is a quantifier-free, invertible interpretation for S_1 of range 0. Since, by Corollary 7.5, $\Phi^F(U) = \overline{F}(U)$ for all structures U over S_1, the interpretation Φ^F, said in a simplified way, replaces every at most 2-element substructure, depending on its isomorphism type, according to the instructions delivered by F.

Let $\mathcal{V}$ be a finite set of finite, connected 1-multigraphs. By Corollary 8.2 $\vec{\Phi^F}(\text{cmb}(\mathcal{V}))$ is preserved under 2-sandwiches (and, indeed, by Corollary 7.14, also under unions of chains).

References

[1] C. C. Chang, H. J. Keisler, *Model Theory*, 3rd ed., Dover Publications, Inc., Mineola, New York, 2012, pp. 306 –313.

[2] C. C. Chang, H. J. Keisler, *Model Theory*, 3rd ed., Dover Publications, Inc., Mineola, New York, 2012, p. 294.

9 Axiomatization and preservation

For a weakly invertible interpretation φ over a set L of relation symbols and a sentence θ in L we explicitly formulate a sentence in L that axiomatizes the class $\varphi(\mathrm{mod}^{\mathrm{L}}(\theta))$ of all structures that φ defines in a model over L of θ, one that axiomatizes the class $\varphi^{\leq i}(\mathrm{mod}^{\mathrm{L}}(\theta))$ of all structures that are φ-derivable in $\leq i$ steps from a model over L of θ and, consequently, also one that axiomatizes $\varphi^{i}(\mathrm{mod}^{\mathrm{L}}(\theta))$ ($i \in \mathbb{N}$). These sentences are further used to establish, for a theory T in L, when $\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$ is axiomatizable.

For a finite set $\mathcal{U}$ of finite, connected structures over L we can infer from the existence of these sentences that the axiomatizability of $\vec{\varphi}(\mathrm{cmb}(\mathcal{U}))$ (the class of all structures that are φ-derivable from a combination of $\mathcal{U}$) implies the decidability of the φ-derivability problem for $\mathrm{cmb}(\mathcal{U})$ and, hence, of $\mathrm{Th}(\vec{\varphi}(\mathrm{cmb}(\mathcal{U})))$.

Finally we are able in this chapter to use the main result of the previous chapter in determining which preservation properties of θ allow us to draw a conclusion about a corresponding preservation property of $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$, if φ is quantifier-free, weakly invertible and $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ axiomatizable. This conclusion yields, of course, a necessary condition for $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ to be axiomatizable, if φ is quantifier-free and weakly-invertible.

For this whole chapter let L be a set of relation symbols.

Let $m \in \mathbb{N}$ and θ be a sentence in L_m. We set for an interpretation φ for L of range r

$$\begin{aligned} \delta_{\theta,\varphi} &= (\zeta_\varphi \wedge \theta\,\varphi); \\ \sigma_{\theta,\varphi} &= (\neg\zeta_\varphi \wedge \theta[c_0,\ldots,c_{m-1} : c_r,\ldots,c_{r+m-1}]). \end{aligned}$$

$(\varphi'(U \restriction \mathrm{L}, u), w) \models \theta$. From the initial assumption $\varphi'(U \restriction \mathrm{L}, u) \neq U \restriction \mathrm{L}$, whence $(U \restriction \mathrm{L}, u) \models \zeta_{\varphi'}$. Thus $U \models \zeta_{\varphi'}[s\colon t][v]$. Again from the initial assumption $U \models \delta_{\theta,\varphi'}[s\colon t][v]$.

(b) Assume $U \models \theta\,\varphi'[s : t][v]$. If $(U \restriction \mathrm{L}, u) \models \zeta_{\varphi'}$, $U \models \zeta_{\varphi'}[s : t][v]$, whence $U \models \delta_{\theta,\varphi'}[s : t][v]$ and, consequently, $U \models \rho_{\theta,\varphi}[s : t][v]$. Otherwise, $\varphi'(U \restriction \mathrm{L}, u) = U \restriction \mathrm{L}$. From the initial assumption $(U \restriction \mathrm{L}, u, w) \models \theta\,\varphi'$ and, therefore, $\varphi'(U \restriction \mathrm{L}, u, w) \models \theta$. Hence $U \models \theta$, whence $U \models \theta[c_0, \ldots, c_{m-1} \colon c_r, \ldots, c_{r+m-1}][s\colon t][v]$. Since φ is invertible, $\varphi(U \restriction \mathrm{L}, u) = U \restriction \mathrm{L}$. Thus $(U \restriction \mathrm{L}, u) \models \neg\zeta_\varphi$, whence $U \models \neg\zeta_\varphi[s\colon t][v]$. We obtain that $U \models \sigma_{\theta,\varphi}[s\colon t][v]$ and, consequently, $U \models \rho_{\theta,\varphi}[s\colon t][v]$.

For the converse, avoiding the trivial case $U \models \delta_{\theta,\varphi'}[s\colon t][v]$, assume $U \models \sigma_{\theta,\varphi}[s\colon t][v]$. Then $\varphi(U \restriction \mathrm{L}, u) = U \restriction \mathrm{L}$ and $U \models \theta$. Since φ is invertible, $\varphi'(U \restriction \mathrm{L}, u, w) = U \models \theta$. Therefore $(U \restriction \mathrm{L}, u, w) \models \theta\,\varphi'$, whence $U \models \theta\,\varphi'[s\colon t][v]$. $\diamondsuit$

Theorem 9.1 (a) *$U \models \rho_{\theta,\varphi}[s\colon t][v]$ iff $U = \varphi(V, u, w)$ for a structure V over* L *with $(V, w) \models \theta$.*

(b) *$U \models (\theta \vee \theta\,\varphi'[s\colon t])[v]$ iff $U \models \theta$ or $U = \varphi(V, u, w)$ for a structure V over* L *with $(V, w) \models \theta$.*

(c) *If φ is invertible, $U \models \theta\,\varphi'[s\colon t][v]$ iff $U = \varphi(V, u, w)$ for a structure V over* L *with $(V, w) \models \theta$.*

Proof. We just prove (a), since (b) and (c) follow easily from (a) and Lemma 9.2. Assume $U \models \delta_{\theta,\varphi'}[s\colon t][v]$. By Lemma 9.1 (a) $(U \restriction \mathrm{L}, u) \in \mathrm{dom}(\varphi')$ and $\varphi'(U \restriction \mathrm{L}, u, w) \models \theta$, which implies, by setting $V = \varphi'(U \restriction \mathrm{L}, u)$, $U = \varphi(V, u, w)$ and $(V, w) \models \theta$.

Theorem 9.2 *The following statements are equivalent for all $i \in \mathbb{N}$:*

(i) *The rank of θ, φ is i.*

(ii) *i is the least $k \in \mathbb{N}$ with $\models (\bigvee_{j\in\mathbb{N}} \xi_j \leftrightarrow \bigvee_{0\leq j\leq k} \xi_j)$.*

(iii) *i is the least elementary bound of θ, φ.*

Proof. (i) $\Rightarrow$ (ii). Left as an exercise for the reader. (Indeed, use Corollary 9.2.) (ii) $\Rightarrow$ (iii). Assume (ii). If the sentence ϕ in L is φ-derivable from some $U \in \mathrm{mod}^{\mathrm{L}}(\theta)$, then ϕ is consistent with $\bigvee_{j\in\mathbb{N}} \xi_j$, whence with $\bigvee_{0\leq j\leq i} \xi_j$. Therefore i is an elementary bound of θ, φ. Assume there is an elementary bound $k < i$ of θ, φ. Because of (ii) $\bigwedge_{0\leq j\leq k} \neg\xi_j$ is consistent with $\bigvee_{j\in\mathbb{N}} \xi_j$, whence φ-derivable from some $U \in \mathrm{mod}^{\mathrm{L}}(\theta)$. Since k is an elementary bound of θ, φ, $\bigwedge_{0\leq j\leq k} \neg\xi_j$ is consistent with $\bigvee_{0\leq j\leq k} \xi_j$, which is a contradiction. This proves that i is the least elementary bound of θ, φ. (iii) $\Rightarrow$ (i). Assume (iii). Obviously the rank of θ, φ is $\geq i$. Assume it is $> i$. Then $\bigwedge_{0\leq j\leq i} \neg\xi_j$ is φ-derivable from some model of θ over L, whence φ-derivable in $\leq i$ steps from some $U \in \mathrm{mod}^{\mathrm{L}}(\theta)$, which implies that it is consistent with $\bigvee_{0\leq j\leq i} \xi_j$, which is a contradiction. This proves that the rank of θ, φ is i. $\diamondsuit$

Corollary 9.4 *The following statements are equivalent:*

(i) *$\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ is axiomatizable.*

(ii) *$\bigvee_{0\leq j\leq i} \xi_j$ axiomatizes $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ for some $i \in \mathbb{N}$.*

all $j \in \mathbb{N}$. With Corollary 7.13 the rank of θ, φ is not ∞. The claim is now immediate from Corollary 9.4, since $r = 0$ in the definition of ξ_j. $\diamondsuit$

Theorem 9.4 *Assume* $1 \leq i \in \mathbb{N}$, φ *is quantifier-free and one (and thus all) of* (i) - (iv) *in Corollary* 9.4 *holds.*

(a) *If* θ *is preserved under* i*-sandwiches,* $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ *is preserved under* $i+1$*-fillings.*

(b) *If* θ *is preserved under* i*-fillings,* $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ *is also preserved under* i*-fillings.*

Proof. Direct consequence of Corollary 9.6, Theorem 8.2 and Theorem 8.3. $\diamondsuit$

Theorem 9.5 *Assume* $1 \leq i \in \mathbb{N}$, φ *is quantifier-free, of range 0 and* θ *is preserved under* i*-sandwiches respectively under chains. Then* $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ *is also preserved under* i*-sandwiches respectively under chains.*

Proof. Direct consequence of Corollary 9.7, Theorem 8.2 and the model theoretical result that a sentence in L belongs to Π_2^{L} iff it is preserved under chains. $\diamondsuit$

As an example let's go back to the interpretation Φ^F in the example at the end of Chapter 8 and let ϑ be any sentence in $\Pi_i^{\mathrm{S}_1}$. Then $i \geq 1$ and, by Theorem 8.2, ϑ is preserved under i-sandwiches. By Theorem 9.5 $\vec{\Phi^F}(\mathrm{mod}^{\mathrm{S}_1}(\vartheta))$ is preserved under i-sandwiches. If ϑ is in $\Sigma_i^{\mathrm{S}_1}$, then, by Theorem 8.3, it is preserved under i-fillings, whence, by Theorem 9.4, $\vec{\Phi^F}(\mathrm{mod}^{\mathrm{S}_1}(\vartheta))$ is preserved under i-fillings.

It is perhaps worth at this point to examine the particular case in which φ is quantifier-free and $\theta \in \Sigma_2^{\mathrm{L}}$ (i. e. θ is existential-universal). In this case Theorem 9.2 can be reformulated in the following way:

Proposition 9.1 *The following statements are equivalent for all $i \in \mathbb{N}$:*

(i) *The rank of θ, φ is i.*

(ii) *i is the least $k \in \mathbb{N}$ with $\models (\bigvee_{j\in\mathbb{N}} \xi_j \leftrightarrow \bigvee_{0\leq j\leq k} \xi_j)$.*

(iii) *i is the least Π_2^{L}-bound of θ, φ.*

Proof. Same as in the proof of Theorem 9.2 by considering that, under the assumption, $\bigwedge_{0\leq j\leq k} \neg\xi_j$ is (equivalent to) a universal-existential sentence. $\diamondsuit$

Proposition 9.2 *If the rank of θ, φ is not ∞, then the φ-derivability problem for* $\mathrm{mod}^{\mathrm{L}}(\theta), \Sigma_2^{\mathrm{L}}$ *is solvable.*

Proof. By Corollary 9.4, if the rank of θ, φ is not ∞, $\bigvee_{0\leq j\leq i} \xi_j$ axiomatizes $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$ for some $i \in \mathbb{N}$. Thus the sentence δ in L is φ-derivable from a model over L of θ iff $\not\models (\bigvee_{0\leq j\leq i} \xi_j \rightarrow \neg\delta)$. If $\delta \in \Sigma_2^{\mathrm{L}}$, then $(\bigvee_{0\leq j\leq i} \xi_j \rightarrow \neg\delta) \in \Pi_2^{\mathrm{L}}$, whence its (logical) validity is decidable. $\diamondsuit$

We now examine more specifically the class $\mathrm{cmb}(\mathcal{U})$ of all combinations of a finite set $\mathcal{U}$ of finite, connected structures over L.

Till the end of this chapter assume that L is finite.

The sentence $\vartheta_{\mathcal{U}}$ was defined in Section 2.5 and satisfies $\mathrm{cmb}(\mathcal{U}) = \mathrm{mod}^{\mathrm{L}}(\vartheta_{\mathcal{U}})$. We set $\xi_j = \exists c_0 \ldots c_{jr-1} \vartheta_{\mathcal{U}}\, \varphi'^j$ $(j \in \mathbb{N})$ and $\mathrm{T} = \mathrm{Th}(\vec{\varphi}(\mathrm{cmb}(\mathcal{U})))$.

We begin with a necessary and sufficient condition for T to be decidable (or equivalently for the φ-derivability problem for $\mathrm{cmb}(\mathcal{U})$ to be solvable):

Then $U \in \vec{\varphi}(\mathrm{cmb}(\mathcal{U}))$ implies $U \in \varphi^{\leq k}(\mathrm{cmb}(\mathcal{U}))$, whence $U \models \bigvee_{j\leq k} \xi_j$. It follows that $\bigvee_{j\leq k} \xi_j$ axiomatizes $\vec{\varphi}(\mathrm{cmb}(\mathcal{U}))$, which yields

$$\phi \in \mathrm{T} \text{ iff } \models (\bigvee_{j\leq k} \xi_j \to \phi).$$

From Proposition 9.3 T is decidable. From Corollary 7.3 the elementary φ-derivability problem for $\mathrm{cmb}(\mathcal{U})$ is solvable. This ends our proof.

Theorem 9.6 *The following statements are equivalent for all $i \in \mathbb{N}$:*

(i) *The rank of* $\mathrm{cmb}(\mathcal{U}), \varphi$ *is i.*

(ii) *i is the least $k \in \mathbb{N}$ with* $\models (\bigvee_{j\in\mathbb{N}} \xi_j \leftrightarrow \bigvee_{0\leq j\leq k} \xi_j)$.

(iii) *i is the least elementary bound of* $\mathrm{cmb}(\mathcal{U}), \varphi$.

(iv) *i is the least elementary bound of* $\mathrm{cmb}(\mathcal{U}), \varphi$ *in the finite.*

(v) *i is the least $k \in \mathbb{N}$ for which* $(\bigvee_{j\in\mathbb{N}} \xi_j \leftrightarrow \bigvee_{0\leq j\leq k} \xi_j)$ *holds in all finite structures over* L.

(vi) *The rank of* $\mathrm{cmb}(\mathcal{U}), \varphi$ *in the finite is i.*

Proof. (i) ⇔ (ii) ⇔ (iii) is Theorem 9.2. (iv) ⇔ (v) ⇔ (vi) is Theorem 9.3. (iii) ⇔ (iv) is Corollary 7.23. ♢

$\Phi^F_{R_1}$ can be written:

$(\gamma_0 \wedge \neg((x_0 = c_0 \wedge x_1 = c_1) \vee (x_0 = c_1 \wedge x_1 = c_0)) \wedge \neg R_1 x_0 x_1) \vee$

$(\gamma_1 \wedge ((x_0 \neq x_1 \wedge R_1 x_0 x_1) \vee (x_0 = x_1 \wedge \neg R_1 x_0 x_0)) \vee$

$(\neg\gamma_0 \wedge \neg\gamma_1 \wedge R_1 x_0 x_1)$.

So far we have investigated the axiomatizability of $\varphi(\mathrm{mod}^{\mathrm{L}}(\theta))$ and $\vec{\varphi}(\mathrm{mod}^{\mathrm{L}}(\theta))$, when θ is a sentence in L. Now we investigate the axiomatizability of $\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$ for a theory T in L. The result obtained leads to the suspect that, more often than not, $\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$ is not axiomatizable.

For a set S of symbols, a theory T in S and a set Σ of formulas $\gamma(x_0, \ldots, x_{n-1})$ in S, we write, following the known model theoretical definition, that Σ is *principal* over T (with respect to n, S) iff there is a formula $\gamma(x_0, \ldots, x_{n-1})$ in S consistent with T that implies in T every formula in Σ (i. e. such that $\mathrm{T} \models (\gamma \rightarrow \phi)$ for all $\phi \in \Sigma$). Σ is *principal* (with respect to n, S) iff it is principal (with respect to n, S) over all complete theories in S consistent with Σ (i. e. over all theories in S consistent with Σ satisfying for all sentences ϕ in S that exactly one of ϕ, $\neg\phi$ follows from the theory).

By the Omitting Type Theorem, if S is countable, T is consistent and Σ is not principal over T (with respect to n, S), then some model of T over S omits Σ (i. e. does not realize Σ).

Let T be a theory in L (that has been assumed to be finite) and $\Sigma = \{\rho_{\gamma,\varphi} \mid \gamma \in \mathrm{T}\}$.

Proposition 9.6 *For all structures U over* L*, if $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$, then U realizes Σ.*

Proof. Assume $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$. Then there is a structure V over L and an r-sequence v to $\mathrm{dom}(V)$ such that $U = \varphi(V, v)$ and $V \models \gamma$ for all $\gamma \in \mathrm{T}$. Hence there is an r-sequence v to $\mathrm{dom}(U)$ such that for all $\gamma \in \mathrm{T}$ there is $V \models \gamma$ over L with $\mathrm{dom}(V) = \mathrm{dom}(U)$ and $U = \varphi(V, v)$. Theorem 9.1 (a) with $m = 0$, $i = r$ implies that there is an r-sequence v to $\mathrm{dom}(U)$ such that $(U, v) \models \rho_{\gamma,\varphi}$ for all $\gamma \in \mathrm{T}$. Thus U realizes Σ. $\diamondsuit$

For principal Σ Proposition 9.6 can be strengthen.

Proposition 9.7 *Suppose that Σ is principal (with respect to r, L). Then for all structures U over L, if $U \models \mathrm{Th}(\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T})))$, then U realizes Σ.*

Proof. Let $U \models \mathrm{Th}(\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T})))$. By Proposition 9.6 $\exists c_0 \ldots c_{r-1} \bigwedge \Delta \in \mathrm{Th}(\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$ for every finite $\Delta \subseteq \Sigma$. Hence $\exists c_0 \ldots c_{r-1} \bigwedge \Delta \in \mathrm{Th}(U)$ for every finite $\Delta \subseteq \Sigma$. By Compactness $\Sigma \cup \mathrm{Th}(U)$ is consistent and $\mathrm{Th}(U)$ is a complete theory in L. By assumption Σ is principal (with respect to r, L) over $\mathrm{Th}(U)$. By definition some formula $\gamma(c_0, \ldots, c_{r-1})$ in L consistent with $\mathrm{Th}(U)$ implies in $\mathrm{Th}(U)$ every formula in Σ. $\mathrm{Th}(U) \models \exists c_0 \ldots c_{r-1}\gamma$, whence $U \models \exists c_0 \ldots c_{r-1}\gamma$. Therefore U realizes Σ. $\diamondsuit$

T is called *φ-uniform* iff for all $\gamma \in \mathrm{T}$, all $V \models \gamma$ over L and all r-sequences v to $\mathrm{dom}(V)$ with $\varphi(V, v) \neq V$ and $\varphi(\varphi(V, v), v) = \varphi(V, v)$ we have $\varphi(V, v) \models \gamma$ or $\varphi(V, v) \not\models \phi$ for all $\phi \in \mathrm{T}$.

We have proven that if $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$, then U realizes Σ. Now we state a condition under which the converse holds, too.

Proposition 9.8 *Assume that* T *is φ-uniform. If U realizes Σ, then $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$.*

L, then $\{(\gamma \wedge \phi) \mid \gamma \in \mathrm{T}\}$ is φ-uniform. By Proposition 9.8 $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}''))$, whence $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$. Conversely, if $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$, then $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}'))$, whence, with Proposition 9.6, U realizes Σ. $\diamondsuit$

Theorem 9.8 *$\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$ is axiomatizable iff Σ is principal (with respect to r, L).*

Proof. Assume Σ is principal and $U \models \mathrm{Th}(\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T})))$. Then $U \models \mathrm{Th}(\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}')))$. By Proposition 9.7 U realizes Σ. By Proposition 9.9 $U \in \varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$. Assume Σ is not principal. Let $\bar{\mathrm{T}}$ be a complete theory in L consistent with Σ over which Σ is not principal (with respect to r, L). $\bar{\mathrm{T}}$ has a model that realizes Σ. By Proposition 9.9 $\mathrm{Th}(\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))) \subseteq \bar{\mathrm{T}}$ (or, more precisely, every sentence in $\mathrm{Th}(\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T})))$ follows from $\bar{\mathrm{T}}$). By the Omitting Types Theorem $\bar{\mathrm{T}}$ has a model over L that omits Σ. Again by Proposition 9.9 some model of $\mathrm{Th}(\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T})))$ is not in $\varphi(\mathrm{mod}^{\mathrm{L}}(\mathrm{T}))$. $\diamondsuit$

References

[1] C. C. Chang, H. J. Keisler, *Model Theory*, 3rd ed., Dover Publications, Inc., Mineola, New York, 2012, p. 220.

[2] W. Hodges, *A shorter model theory*, Cambridge University Press, Cambridge, 1997, p. 247, Exercise 9.

10 Local interpretations

The locality property is the last bit we need to narrow down interpretations to regular and reactional ones. As written in the preamble of Chapter 7 the name "regular" is derived from the latin word "regula", which means rule. The locality property is inspired by the shift operation of Chapter 3, which modifies an n-multigraph only within the positions at which it is applied. Quantifier-free, local interpretations have a rather simple, in a way, graphic model theoretical characterization by means of replacements, which, in their turn, allow to build a correspondence between $\mathcal{S}$-shift operations, for a finite set $\mathcal{S}$ of finite n-rules, and interpretations. If φ is a quantifier-free interpretation for S_n, defined at the beginning of Chapter 2, with the property that all $H \in \varphi(G)$ are similar to G for all n-multigraphs G, then locality ensures that there is a finite set $\mathcal{S}$ of finite n-rules such that $\varphi(G)$ is the set of all $\mathcal{S}$-shifts of G for every n-multigraph G.

Let L be a set of relation symbols, φ an interpretation for L of range r and $n \in \mathbb{N}$. φ is called *n-local* iff $U \models (Rx_0 \dots x_{\nu_R-1} \leftrightarrow \varphi_R)[u]$ for all $R \in \mathrm{L}$, all structures U over L_r and all ν_R-sequences u to $\mathrm{dom}(U)$ with $\{u_0, \dots, u_{\nu_R-1}\} \not\subseteq \mathrm{nb}^n_{_U}(\{c^U_0, \dots, c^U_{r-1}\})$. In this definition we use the notation for $\mathrm{nb}^n_{_U}$ given at the beginning of Chapter 6 (i. e. $\mathrm{nb}^n_{_U} = \mathrm{nb}^n_{\mathrm{gf}(U)}$). φ is *local* iff it is 0-local. Until the beginning of Section 10.1 assume that φ is n-local. We maintain the meaning of the expansion (U, u) of U given in Chapter 7.

Proposition 10.1 *If $n = 0$ and φ is weakly invertible, then φ' is n-local.* $\diamondsuit$

Proposition 10.1 does not hold by omitting $n = 0$ in the premise. The inverse of the following 1-local, weakly invertible interpretation ψ for $\{R\}$ (R 2-placed relation symbol) of range 1 is not 1-local:

$$\begin{aligned}\psi_R = \quad & (((\neg Rc_0c_0 \wedge \forall x_0(Rx_0x_0 \to (Rx_0c_0 \wedge Rc_0x_0))) \quad \to \quad (\neg(x_0 = c_0 \wedge Rx_1x_1)\wedge \\ & \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \neg(x_1 = c_0 \wedge Rx_0x_0) \wedge Rx_0x_1)) \\ & \wedge \\ & (\neg(\neg Rc_0c_0 \wedge \forall x_0(Rx_0x_0 \to (Rx_0c_0 \wedge Rc_0x_0))) \quad \to \quad Rx_0x_1)).\end{aligned}$$

In every structure over $\{c_0, R\}$, where c_0 does not have R with itself and all elements that do, have R with c_0 and c_0 with them, ψ deletes precisely all edges, determined by R, between c_0 and an element that has R with itself. Its inverse is given by

$$\begin{aligned}\psi'_R = \quad & (((\neg Rc_0c_0 \wedge \forall x_0(Rx_0x_0 \to (\neg Rx_0c_0 \wedge \neg Rc_0x_0))) \quad \to \quad ((x_0 = c_0 \wedge Rx_1x_1)\vee \\ & \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (x_1 = c_0 \wedge Rx_0x_0) \vee Rx_0x_1)) \\ & \wedge \\ & (\neg(\neg Rc_0c_0 \wedge \forall x_0(Rx_0x_0 \to (\neg Rx_0c_0 \wedge \neg Rc_0x_0))) \quad \to \quad Rx_0x_1)).\end{aligned}$$

Proposition 10.2 *Let U, V be structures over* L *with disjoint domains, $W = U \oplus V$ and u an r-sequence to* $\mathrm{dom}(U)$.

(a) $\varphi(W, u) = \varphi(W, u)|\mathrm{dom}(U) \oplus V$.

(b) *If φ is quantifier-free, $\varphi(W, u) = \varphi(U, u) \oplus V$.*

Proof. (a) Assume that $R \in \mathrm{L}$ and v is a $\nu_{\mathbf{R}}$-sequence to $\mathrm{dom}(W)$ with $\{v_0, \ldots, v_{\nu_{\mathbf{R}}-1}\} \not\subseteq \mathrm{dom}(U)$. Since

$$\{v_0, \ldots, v_{\nu_R-1}\} \not\subseteq \mathrm{nb}^n_W(\{u_0, \ldots, u_{r-1}\})$$

and φ is n-local,

$$R^{\varphi(W,u)}(v_0, \dots, v_{\nu_R - 1}) \quad \text{iff} \quad R^W(v_0, \dots, v_{\nu_R - 1}).$$

(b) From Proposition 7.1 we obtain

$$\varphi(W, u)|\mathrm{dom}(U) = \varphi(U, u).$$

Now use (a). $\diamondsuit$

Proposition 10.3 *Let $n \leq 1$ and ψ be an n-local interpretation for* L *of range s. Then $\psi\,\varphi$ is n-local.*

Proof. Let $R \in \mathrm{L}$, U be a structure over L_{r+s}, u a ν_R-sequence to $\mathrm{dom}(U)$ with $\{u_0, \dots, u_{\nu_R - 1}\} \not\subseteq \mathrm{nb}^n_U(\{c^U_0, \dots, c^U_{r+s-1}\})$. Abbreviate $U' = U \restriction \mathrm{L}_r$. Using Theorem 7.4 we have:

$$\begin{aligned} &U \models (\psi\,\varphi)_R[u] \qquad \text{iff} \quad U \models \psi_R\,\varphi[u] \quad \text{iff} \quad \varphi(U) \models \psi_R[u] \quad \text{iff} \\ &(\varphi(U'), (c^U_{r+i})_{0 \leq i < s}) \models \psi_R[u]. \end{aligned} \tag{1}$$

By Proposition 2.3(a) there is $a \in \{u_0, \dots, u_{\nu_R - 1}\}$ with

$$a \notin (\mathrm{nb}^n_U(\{c^U_0, \dots, c^U_{r-1}\}) \cup \mathrm{nb}^n_U(\{c^U_r, \dots, c^U_{r+s-1}\})). \tag{2}$$

Therefore, keeping in mind that φ is n-local, for any $Q \in \mathrm{L}$, any ν_Q-sequence v to $\mathrm{dom}(U)$ with $a \in \{v_0, \dots, v_{\nu_Q - 1}\}$

$$U' \models \varphi_Q[v] \text{ iff } Q^U(v_0, \dots, v_{\nu_Q - 1}). \tag{3}$$

where $r = 4k + \max\{|\mathrm{dom}(K)| - |\{u_0, \ldots, u_{4k-1}\}| \mid (K, u) \in \mathcal{S}\}$ and $v_{K,u}$ is a surjective sequence u, a to $\mathrm{dom}(K)$ for some m-sequence a with $m = |\mathrm{dom}(K)| - |\{u_0, \ldots, u_{4k-1}\}|$ $((K, u) \in \mathcal{S})$.

Theorem 10.1 *$\sigma|\delta$ is a reactional interpretation for S_n and H is an $\mathcal{S}$-shift of G iff $\sigma|\delta$ interprets H in G for all n-multigraphs G, H.*

Proof. Follows from Lemma 10.1(f) and Proposition 3.10. $\diamondsuit$

It is easy to establish that the range of $\sigma|\delta$ is

$4k + \max\{|\mathrm{dom}(K)| - |\{u_0, \ldots, u_{4k-1}\}| \mid (K, u) \in \mathcal{S}\}$, if $k > 0$ and $\mathcal{S} \neq \emptyset$;

$4k$, if $k > 0$ and $\mathcal{S} = \emptyset$;

1, if $k = 0$.

In order to obtain two significant corollaries of Theorem 10.1, we start from $\mathcal{T}_0 = (\tilde{\mathrm{S}}_{14}, \rho_0)$, $\mathcal{I}_0 = (\tilde{\mathrm{S}}_{14}, \sigma_0), \mathcal{H}$ and $H_0 := \sum \mathcal{H}$, used in Corollary 5.3. We set δ_0 to be the value of the previously defined δ with $\mathcal{S} = \mathrm{arp}_{14}(\mathcal{T}_0)$ and δ_1 the value of δ with $\mathcal{S} = \mathrm{arp}_{14}(\mathcal{I}_0)$ (in both cases $k = 2$).

With Theorem 10.1 $\sigma|\delta_0$ and $\sigma|\delta_1$ are reactional interpretations for S_{14} of range ≤ 12 for which

H is an $\mathrm{arp}_{14}(\mathcal{T}_0)$-shift of G iff $\sigma|\delta_0$ interprets H in G and

H is an $\mathrm{arp}_{14}(\mathcal{I}_0)$-shift of G iff $\sigma|\delta_1$ interprets H in G

for all 14-multigraphs G, H. Corollary 5.3 yields

Corollary 10.1 *The $\sigma|\delta_0$-synthesizability problem for the class of finite $\mathcal{U} \subseteq \mathcal{G}_{d_{14}} \cap \mathcal{G}^1$, $\mathrm{srp}_{14}(\emptyset)$, where $\emptyset$ is the empty word, and the $\sigma|\delta_1$-synthesizability problem for $\mathcal{H}$ (by Corollary 7.1 also for $\{H_0\}$), $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1 \cap \mathcal{G}^{\mathrm{conn}}$ are unsolvable.* $\diamondsuit$

With Corollary 9.8 and Corollary 9.9 we obtain

Corollary 10.2 *$\overrightarrow{\sigma|\delta_0}(\mathrm{cmb}(\mathcal{H}))$ and $\overrightarrow{\sigma|\delta_0}(\mathrm{cmb}(\{H_0\}))$ (both $\subseteq \mathcal{G}_{d_{14}} \cap \mathcal{G}^1$) are not first-order axiomatizable and are not closed under ultraproducts.* $\diamondsuit$

With the introduction of replacements in the next section, we will be able to show that for all finite sets $\mathcal{S}$ of finite n-rules there is a reactional interpretation φ for S_n such that H is an $\mathcal{S}$-shift of G iff φ interprets H in G for all n-multigraphs G, H. We will also be able to prove its vice versa: For every quantifier-free, local interpretation φ for S_n, carrying any n-multigraph at any position into a similar n-multigraph, there is a finite set $\mathcal{S}$ of finite n-rules such that H is an $\mathcal{S}$-shift of G iff φ interprets H in G for all n-multigraphs G, H.

10.2 Replacements

We will need the definition of $e_{U,V}$ and of $\Delta_{U,u}$, given in Chapter 1, and of (U, u) given at the beginning of Chapter 7. Recall that we do not distinguish between equivalent interpretations. Let L be a set of relation symbols and $r \in \mathbb{N}$.

An *r-move* for L is a pair (A, B), where A is a canonical structure over L_r and B a structure over L with $\mathrm{dom}(B) = \mathrm{dom}(A)$. The r-move $(A, A\restriction\mathrm{L})$ for L is called *trivial.*

The r-moves (A, B), (A', B') for L are *equivalent* (or (A, B) is *equivalent* to (A', B')) iff there is f: $\mathrm{dom}(A) \to \mathrm{dom}(A')$ that is an isomorphism from A to A' and from B to B', or, said differently, iff $A \cong A'$ and $e_{A,A'}$ is an isomorphism from B to B'. The sets $\mathcal{P}, \mathcal{R}$ of r-moves for L are *equivalent* (or $\mathcal{P}$ is *equivalent* to $\mathcal{R}$) iff every non-trivial element in $\mathcal{P}$ is equivalent to an element in $\mathcal{R}$ and vice versa.

Let U, V be structures over L and u an r-sequence to $\mathrm{dom}(U)$. An r-move (A, B) for L *carries* U into V at u iff A is embedded into (U, u) and V is the U-extension of B by $e_{A,(U,u)}$. A set $\mathcal{R}$ of r-moves for L *carries* U into V at u (or V is an *application* of $\mathcal{R}$ to U at u) iff some $(A, B) \in \mathcal{R}$ carries U into V at u. $\mathcal{R}$ *carries* U into V (or V is an *application* of $\mathcal{R}$ to U) iff it carries U into V at some r-sequence u to $\mathrm{dom}(U)$.

Proposition 10.7 *If the r-moves (A, B) and (A', B') for* L *carry U into V at u, then they are equivalent.*

Proof. A and A' are embedded into (U, u). Thus the composition $f := e_{(U,u),A'} \circ e_{A,(U,u)}$ is an isomorphism from A to A'. But $e_{A,(U,u)}$ is an isomorphism from B to $V|\{u_0, \ldots, u_{r-1}\}$ and $e_{(U,u),A'}$ from $V|\{u_0, \ldots, u_{r-1}\}$ to B'. Hence f is an isomorphism from B to B'. $\diamondsuit$

An *r-replacement* for L is a set $\mathcal{R}$ of r-moves for L for which (A, B) is equivalent to (A', B') whenever $A \cong A'$ for all (A, B), $(A', B') \in \mathcal{R}$. A *replacement* for L is an r-replacement for L for some $r \in \mathbb{N}$. A *replacement* is a replacement for some set of relation symbols.

Proposition 10.8 *If $\mathcal{R}$ is an r-replacement for* L*, U a structure over* L *and u an r-sequence to* $\mathrm{dom}(U)$*, then there is at most one structure into which $\mathcal{R}$ carries U at u.*

Proof. Immediate from the definition of r-replacement and of U-extension of B by f. $\diamondsuit$

Let L be a finite set of relation symbols and $r \in \mathbb{N}$.

To every local interpretation φ for L of range r we associate a maximal set $\mathcal{R}$ of non-trivial, (pairwise) non-equivalent r-moves (A, B) for L for which there is an extension $U \supseteq A$ with $\varphi(U) \supseteq B$. $\mathcal{R}$ is finite and unique up to equivalence. We denote it by $\mathcal{M}^\varphi$. Obviously $\mathcal{M}^\varphi$ carries U into $\varphi(U, u)$ at u for all structures U over L and all r-sequences u to $\mathrm{dom}(U)$ with $\varphi(U, u) \neq U$. For quantifier-free φ the converse holds, too:

Proposition 10.9 *Assume that φ is quantifier-free and local. Then $\mathcal{M}^\varphi$ is a replacement and for all structures $U \neq V$ over* L*, all r-sequences u to* $\mathrm{dom}(U)$*, if $\mathcal{M}^\varphi$ carries U into V at u, then $V = \varphi(U, u)$.*

Proof. As a consequence of Proposition 7.1, $\varphi(A) = B$ for all $(A, B) \in \mathcal{M}^\varphi$. This proves that $\mathcal{M}^\varphi$ is a replacement, because for any structures W, Y over L_r, if f is an isomorphism from W to Y, then f is an isomorphism from $\varphi(W)$ to $\varphi(Y)$. Suppose $\mathcal{M}^\varphi$ carries U into V at u. Then there is $(A, B) \in \mathcal{M}^\varphi$ for which A is embedded into (U, u) and V is the U-extension of B by $e_{A,(U,u)}$. Since $B = \varphi(A)$, $e_{A,(U,u)}$ (that is the isomorphism from A to $(U, u)|\{u_0, \ldots, u_{r-1}\}$) is an isomorphism from B to $\varphi((U, u)|\{u_0, \ldots, u_{r-1}\}) = \varphi(U, u)|\{u_0, \ldots, u_{r-1}\}$. Therefore $e_{A,(U,u)}$ is an embedding from B into $\varphi(U, u)$. Since φ is local, $\varphi(U, u) = V$. $\diamondsuit$

of G, with $\mathcal{S}$ a finite set of finite n-rules, and the class of the relations that hold for the n-multigraphs G, H iff φ interprets H into G, where φ is a reactional interpretation for S_n, are the same.

Theorem 10.3 *For every finite set $\mathcal{S}$ of finite n-rules there is a non-multigraph preserving, reactional interpretation φ for S_n and for every reactional interpretation φ for S_n there is a finite set $\mathcal{S}$ of finite n-rules such that for all n-multigraphs G, H*

H is an $\mathcal{S}$-shift of G iff φ carries G into H.

Proof. Since $\mathrm{sh}(G, \emptyset) = G$, with Proposition 10.19, it is enough to prove the theorem for $G \neq H$. Let $\mathcal{S}$ be a finite set of finite n-rules and $\mathcal{S}'$ the set of the at least 1-fold n-rules in $\mathcal{S}$. Assume that all cardinalities of $\mathrm{dom}(K)$ with $(K, a) \in \mathcal{S}'$ are $\leq m$ and all i for which there is an i-fold n-rule in $\mathcal{S}'$ are $\leq k$. Set $r = m + 4(k-1)$. From each j-fold n-rule $(K, a) \in \mathcal{S}'$ form an r-move $(\bar{K}, \mathrm{sh}(K, a))$ for S_n, where $\bar{K} \restriction \mathrm{S}_n = K$, $c_i^{\bar{K}} = a_i$ $(0 \leq i < 4j)$, $c_{4j}^{\bar{K}} = \ldots = c_{4k-1}^{\bar{K}}$. Now build the set $\mathcal{R}$ of all r-moves formed from some n-rule in $\mathcal{S}'$. A simple examination shows that $\mathcal{R}$ and $\mathcal{R}'$ are replacements $(\mathrm{sh}^{-1}(\mathrm{sh}(K, a), a) = K)$ and that for all n-multigraphs G and all structures $V \neq G$ over S_n

V is an $\mathcal{S}$-shift of G iff $\mathcal{R}$ carries G into V.

By Proposition 10.11 and Proposition 10.16 $\Psi^{\mathcal{R}}$ is a regular interpretation for S_n of range r such that for all structures $U \neq V$ over S_n and all r-sequences u to $\mathrm{dom}(U)$

$\Psi^{\mathcal{R}}(U, u) = V$ iff $\mathcal{R}$ carries U into V at u.

An examination of the proof of Theorem 10.3 shows that for its second correspondence the weak invertibility of φ is not needed. As a consequence we have actually proven a slight strengthening of Corollary 10.7 (a).

Proposition 10.21 *For every quantifier-free, local, similarity preserving interpretation φ for S_n there is a reactional, non-multigraph preserving interpretation for S_n that, for all n-multigraphs G, H, carries G into H iff φ carries G into H.* $\diamondsuit$

Proposition 10.21 and Corollary 10.7 (b) yield a strengthening of Corollary 10.7 (b) itself.

Proposition 10.22 *For every quantifier-free, local, similarity preserving interpretation φ for S_n there is a reactional interpretation ψ for S_n with $\psi' = \psi$ that, for all n-multigraphs G, H, carries G into H iff φ carries G into H or H into G.* $\diamondsuit$

11 Reduction to a case of the logical decision problem

In this chapter, under the assumption that φ is quantifier-free, the φ-synthesizability problem (for $\mathcal{C}_0,\ \mathcal{C}_1$) , stated in Chapter 7, is reduced to the finite satisfiability problem for a set of first-order sentences (depending, of course, on $\varphi, \mathcal{C}_0, \mathcal{C}_1$). This reduction delivers gratuitously an undecidability result for the finite satisfiability problem of two classes of sentences defined in a standard way ("almost" completely through the prefixes).

Let L be a finite set of relation symbols, φ an interpretation for L of range r and δ a sentence in L. Notice immediately that the structure V over L is a φ-product of U iff Δ_V is φ-derivable from U .

A *φ-derivation tree* (of δ from U_0) is a sequence $U_0, \ldots, U_l$ of structures over L (with $U_l \models \delta$) where for every $0 < i \leq l$ there are $0 \leq j < i$ and $V \supseteq U_i$ such that φ carries U_j into V.

Suppose that φ is quantifier-free and δ is existential.

Proposition 11.1 *δ is φ-derivable from U_0 iff there is a φ-derivation tree of δ from U_0.*

Proof. $\Rightarrow$ is obvious. $\Leftarrow$: By induction on the length of the φ-derivation tree. The case of length 1 is trivial. In passing from l to $l+1$, let $U_0, \ldots, U_{l+1}$ be a φ-derivation tree with $U_{l+1} \models \delta$. There are $0 \leq i \leq l$ and $V \supseteq U_{l+1}$ such that φ carries U_i into

V. Indeed there is a φ-derivation tree of the existential sentence Δ_{U_i} from U_0 of length $\leq l$. By induction there is a φ-derivation $U'_0, \ldots, U'_k$ with $U'_0 = U_0$ and $U'_k \models \Delta_{U_i}$. This implies $U_i \subseteq U'_k$. With Proposition 7.1 φ carries U'_k into a $\overline{V} \supseteq V$. Since δ is existential, $\overline{V} \models \delta$. $\diamondsuit$

Let M be a 1-placed relation symbol and $\leq, Q, F, X_0, X_1, \ldots$ be 2-placed relation symbols not in L.

To a finite set $\mathcal{U}$ of finite, connected structures over L we effectively associate a sentence $\Phi = (\phi_0 \wedge \phi_1)$ in $\mathrm{L} \cup \{M, \leq, Q, F, X_0, \ldots, X_{r-1}\}$, where ϕ_0 is universal and ϕ_1 is prenex with prefix type $\forall\exists^*$, that axiomatizes in the finite the range of a one-to-one (up to isomorphism[6]) representation of the φ-derivation trees of δ from a substructure of a finite combination of $\mathcal{U}$. Φ is also of the form $(\phi \wedge \bigwedge_{0 \leq i \leq r} \forall x \exists y X_i xy)$, where ϕ is an existential-universal sentence.

Let $\mathcal{C}$ be the class of all substructures of the combinations of $\mathcal{U}$ and

$$l = \max\{|\mathrm{dom}(U)| \mid U \in \mathcal{U}\} + 1.$$

In order to obtain Φ we effectively associate to $\mathcal{U}$ a universal sentence $\forall x_0 \ldots \forall x_{l-1} \alpha_{\mathcal{U}}$, $\alpha_{\mathcal{U}}$ quantifier-free, in L that axiomatizes $\mathcal{C}$.

Proposition 11.2 *Let* T *be the set of all universal sentences in* L *with l quantifiers that hold in all structures in $\mathcal{C}$. Then* T *axiomatizes $\mathcal{C}$.*

[6] The φ-derivation tree $U_0, \ldots, U_l$ is *isomorphic* to the φ-derivation tree $V_0, \ldots, U_m$ iff $l = m$ and there is $f\colon \mathrm{dom}(U_0) \to \mathrm{dom}(V_0)$ for which $f|\mathrm{dom}(U_i)$ is an isomorphism from U_i to V_i for all $0 \leq i \leq l$.

Proof. Let V be a structure over L that satisfies T. Then every at most l-element substructure of V belongs to $\mathcal{C}$. Otherwise there would be a universal sentence in L with l quantifiers that holds in all structures of $\mathcal{C}$ but fails in V, hence a $\gamma \in$ T with $V \not\models \gamma$, which is a contradiction.

Suppose that A is a component of V. A is closed in gf(V). By Proposition 2.21(a), gf$(V|A) =$ gf$(V)|A$. By Proposition 2.14 gf$(V|A)$ is connected. By Proposition 2.18 and again Proposition 2.21(a) there is an $\leq l$-element $B \subseteq A$ for which $V|B$ is connected. With Proposition 2.24, since $V|B \in \mathcal{C}$, $V|B$ is embedded into some $U \in \mathcal{U}$, which contradicts $|\mathrm{dom}(U)| < l$. Hence every component of V has cardinality $< l$. Thus it belongs to $\mathcal{C}$. This proves $V \in \mathcal{C}$. $\diamondsuit$

$\bigwedge T$ is logically equivalent to a universal sentence with l quantifiers. The next proposition shows that the association of $\bigwedge T$ to $\mathcal{U}$ is computable and allows us to set $\forall x_0 \dots \forall x_{l-1} \alpha_{\mathcal{U}} = \bigwedge T$.

Proposition 11.3 *A universal sentence in* L *with l quantifiers holds in all structures of $\mathcal{C}$ iff it holds in every l-combination of $\mathcal{U}$.*

Proof. Indeed every at most l-element substructure of a combination of $\mathcal{U}$ is embedded into an l-combination of $\mathcal{U}$. A structure V over L satisfies all universal first-order sentences with k quantifiers that hold in all structures of a set $\mathcal{V}$ of structures over L iff every at most k-element substructure of V is embedded into some $W \in \mathcal{V}$. $\diamondsuit$

Set $\delta = \exists x_0 \dots x_m \zeta(x_0, \dots, x_m)$, ζ quantifier-free. We shorten $(x \leq y \wedge x \neq y)$ by

$(G, u) \models \gamma[R_i st\colon (s = t \wedge R_i ss) \ \ (s, t \text{ terms in } \{c_0, \ldots, c_r\},\ 2 \le i \le n)][a_0, \ldots, a_{m-1}]$.

Obviously, since $\mathrm{arp}_{14}(\mathcal{T}_0)$ and $\mathrm{arp}_{14}(\mathcal{I}_0)$ are sets of 1-bound 14-rules, for $j = 0, 1$

$$\begin{aligned}&\text{if } G \text{ is a 1-bound 14-multigraph and } \varphi_j \text{ interprets } H \text{ in } G,\\ &\text{then } H \text{ is a 1-bound 14-multigraph.}\end{aligned} \tag{9}$$

Let G, H be 1-bound 14-multigraphs, U a structure over $\{R_1, P_2, \ldots, P_{14}\}$ and $j = 0$ or $j = 1$. For the sake of precision, we make a few straightforward remarks regarding the coding crg. From (8) it is easy to infer that if U is ψ_j-derivable from $\mathrm{crg}(G)$, then $U = \mathrm{crg}(K)$ for some 1-bound 14-multigraph K. With (9) it follows that H is φ_j-derivable from G iff $\mathrm{crg}(H)$ is ψ_j-derivable from $\mathrm{crg}(G)$. Given that $H \subseteq G$ iff $\mathrm{crg}(H) \subseteq \mathrm{crg}(G)$, we obtain

$$H \text{ is a } \varphi_j\text{-product of } G \text{ iff } \mathrm{crg}(H) \text{ is a } \psi_j\text{-product of } \mathrm{crg}(G). \tag{10}$$

We go back to the set $\mathcal{H}$, defined in Section 5.2 and used in Corollary 5.3 as well as in Corollary 10.1, which is a finite set of at most 6-element structures in $\mathcal{G}_{d_{14}} \cap \mathcal{G}^1 \cap \mathcal{G}^{\mathrm{conn}}$ and set $\mathcal{H}' = \{\mathrm{crg}(G) \mid G \in \mathcal{H}\}$. Thus $\mathcal{H}'$ is a finite set of at most 6-element, connected structures over $\{R_1, P_2, \ldots, P_n\}$. Again we state a few elementary facts about crg. For every combination set $\mathcal{G}$ of $\mathcal{H}$ and every combination set $\mathcal{G}'$ of $\mathcal{H}'$

$$\begin{aligned}&\mathrm{crg}(\textstyle\sum \mathcal{G}) = \sum\{\mathrm{crg}(G) \mid G \in \mathcal{G}\},\\ &\{\mathrm{crg}(G) \mid G \in \mathcal{G}\} \text{ is a combination set of } \mathcal{H}' \text{ and}\\ &\mathcal{G}' = \{\mathrm{crg}(G) \mid G \in \mathcal{F}\} \text{ for a combination set } \mathcal{F} \text{ of } \mathcal{H}.\end{aligned} \tag{11}$$

Corollary 10.1 states that

(a) no procedure decides for all finite $\mathcal{F} \subseteq \mathcal{G}_{d_{14}} \cap \mathcal{G}^1$ whether $\mathrm{srp}_{14}(\emptyset)$, with $\emptyset$ the empty word, is a φ_0-product of a combination of $\mathcal{F}$ and

(b) no procedure decides for all $H \in \mathcal{G}_{d_{14}} \cap \mathcal{G}^1 \cap \mathcal{G}^{\mathrm{conn}}$ whether H is a φ_1-product of a combination of $\mathcal{H}$.

In (a) we can indeed assume that the 14-multigraphs in $\mathcal{F}$ have pairwise disjoint domains. With Corollary 7.2 we obtain that no procedure decides for all finite $\mathcal{F} \subseteq \mathcal{G}_{d_{14}} \cap \mathcal{G}^1$ with pairwise disjoint domains whether $\mathrm{srp}_{14}(\emptyset)$ is a φ_0-product of a combination of $\sum \mathcal{F}$ and therefore that no procedure decides for all finite $G \in \mathcal{G}_{d_{14}} \cap \mathcal{G}^1$ whether $\mathrm{srp}_{14}(\emptyset)$ is a φ_0-product of a combination of G. Finally with (10) we can state that

(a') no procedure decides for all finite U over $\{R_1, P_2, \ldots, P_{14}\}$ whether $\mathrm{crg}(\mathrm{srp}_{14}(\emptyset))$ is a ψ_0-product of a combination of U.

(b), (10) and (11) yield the result:

(b') No procedure decides for all finite U over $\{R_1, P_2, \ldots, P_{14}\}$ whether U is a ψ_1-product of a combination of $\mathcal{H}'$.

(a'), (b') and (7) imply that the finite satisfiability problem for the sets of sentences

$$\Sigma_0 = \{\Phi(\psi_0, \Delta_{\mathrm{crg}(\mathrm{srp}_{14}(\emptyset))}, \{U\}) \,|\, U \text{ finite structure over } \{R_1, P_2, \ldots, P_{14}\}\},$$

$$\Sigma_1 = \{\Phi(\psi_1, \Delta_U, \mathcal{H}') \,|\, U \text{ finite structure over } \{R_1, P_2, \ldots, P_{14}\}\},$$

where Φ was defined through (1) - (6), is undecidable.

Let $\mathbf{P}_0 = [\forall^* \wedge \exists^2, (14,17)]_=$, $\mathbf{P}_1 = [\forall^{16} \wedge \exists^*, (14,17)]_=$. $\mathbf{P}_0$ is the class of all conjunctions of a relational, universal sentence (allowing equality) and a relational, existential sentence with 2 quantifiers (still allowing equality), that have at most 14 1-placed and 17 2-placed relation symbols and no j-placed symbols for $j \neq 1,2$. $\mathbf{P}_1$ is the class of all conjunctions of a relational, existential sentence (allowing equality) and a relational, universal sentence with 16 quantifiers (still allowing equality), that again have at most 14 1-placed and 17 2-placed relation symbols and no j-placed symbols for $j \neq 1,2$. For an exact explanation of the class notation $[P,(),()]$ refer to [3]. Σ_0 respectively Σ_1 are contained in the classes $\mathbf{P}_0 \wedge \bigwedge_{0\leq i<13} \forall x \exists y S_i xy$ respectively $\mathbf{P}_1 \wedge \bigwedge_{0\leq i<13} \forall x \exists y S_i xy$, S_i 2-placed relation symbol ($0 \leq i < 13$), of all conjunctions of the sentence $\bigwedge_{0\leq i<13} \forall x \exists y S_i xy$ and a sentence in $\mathbf{P}_0$ respectively in $\mathbf{P}_1$. These facts prove the following theorem:

Theorem 11.1 *The finite satisfiability problems for the classes* $\mathbf{P}_0 \wedge \bigwedge_{0\leq i<13} \forall x \exists y S_i xy$ *and* $\mathbf{P}_1 \wedge \bigwedge_{0\leq i<13} \forall x \exists y S_i xy$ *are undecidable.* $\diamondsuit$

Regarding the decision problem recall that the class $[\exists\forall^*] \wedge \forall x \exists y Sxy$ (S 2-placed relation symbol) is the (undecidable) Ackermann's reduction class for the (classical) satisfiability problem [1], [7]. $[\exists\forall^*]$ allows all relation symbols with no number bound, but not the equality. It follows from the undecidability of the Gurevich class $[\forall,(0),(2)]_=$, refer to [4], [9], that $\mathbf{P}_2 := [\forall^*,(0,2)]_= \wedge \forall x \exists y S_0 xy \wedge \forall x \exists y S_1 xy$ is undecidable as well. Therefore the satisfiability problem for the first class in Theorem 11.1 is unsolvable. The Gurevich class however (and, as a consequence, $\mathbf{P}_2$) does not have the finite satisfiability property,

$$\forall x(ffgx = fx \wedge fgx \neq x) \ (f, g \text{ 1-placed function symbols})$$

being an axiom of infinity. For an explanation why, see [5]. It is also important to point out that the class $[\exists^*\forall^*, (\omega, 1)]_= \ \wedge \ \forall x \exists y Sxy$ has been proven decidable for finite satisfiability by Kostyrko [2], [8].

We conclude this chapter with two open questions. Let S_i be a 2-placed relation symbol ($i \in \mathbb{N}$). Set

$\mathbf{Q}_{0,j} = [\forall^* \wedge \exists^2, (\omega, j)]_= \ \wedge \ \bigwedge_{0 \leq i < j} \forall x \exists y S_i xy$,

$\mathbf{Q}_{1,j} = [\forall^j \wedge \exists^*, (\omega, \omega)]_= \ \wedge \ \bigwedge_{i \in \mathbb{N}} \forall x \exists y S_i xy$,

($j \in \mathbb{N}$). By Kostyrko's result the finite satisfiability problem for $\mathbf{Q}_{0,1}$ is decidable. Since $\mathbf{Q}_{1,1}$ is contained in the Shelah class [6], its finite satisfiability problem is decidable as well. By Theorem 11.1 the finite satisfiability problem for $\mathbf{Q}_{0,17}$ and for $\mathbf{Q}_{1,16}$ are undecidable. This leaves us with the open questions:

Which is the largest $j \in \mathbb{N}$ for which $\mathbf{Q}_{0,j}$ is decidable?

Which is the largest $j \in \mathbb{N}$ for which $\mathbf{Q}_{1,j}$ is decidable?

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12 From $\mathcal{S}$-synthesis to organic chemical synthesis

In this chapter words and expressions from the vocabulary of organic chemistry are defined in terms of the graph theoretical definitions given in Chapter 2 and 3. These definitions will allow to clarify the intended organic chemical meaning of the graph theoretical definitions and to translate into the chemical language several statement previously obtained.

The words and expressions from the vocabulary of organic chemistry are defined with parameters using the three distinct symbols $+$, $-$, $\bullet$. The parameters are:

$m \in \mathbb{N}$,

a surjective function, called *multiplicity*, from a set, whose elements are called *bonds*, to $\{1, \ldots, m\}$ (a bond of multiplicity $1, 2, 3, 4, > 1$ is called respectively *single, double, triple, quadruple, multiple*),

a set $\mathrm{I} \subseteq \{+, -, \bullet\}$, whose elements are called *implicit symbols* ,

a finite set A, with $\mathrm{A} \cap \mathrm{I} = \emptyset$ and $\mathrm{A} \cup \mathrm{I} \neq \emptyset$, whose elements are called *atomic symbols*

and, finally, a function, called *valence*, from $\mathrm{A} \cup \mathrm{I}$ to $\mathbb{N}$, assigning 1 to every implicit symbol (not to be confused with the valence in an n-multigraph).

We call an element of $\mathrm{A} \cup \mathrm{I}$ (i. e. that is either an atomic or an implicit symbol) a *building symbol*.

For the rest of this chapter let $n+1$ be the number of building symbols (i. e. $n = |\mathrm{A} \cup \mathrm{I}| - 1$) , s be a bijection from $\{0, \ldots, n\}$ to the set $\mathrm{A} \cup \mathrm{I}$ of building symbols and $d\colon \{0, \ldots, n\} \to \mathbb{N}$ satisfy the condition that $d(i)$ is the valence of $s(i)$ $(0 \leq i \leq n)$.

We call an element of $\mathcal{G}_{\leq d} \cap \mathcal{G}^m \cap \mathcal{G}^{\mathrm{conn}}$ an *arrangement*. Hence an arrangement is a finite, connected, m-bound n-multigraph A with $\deg_A(a) \leq d(\mathrm{val}_A(a,a))$ $(a \in \mathrm{dom}(A))$. Since $\mathcal{G}_{\leq d} \cap \mathcal{G}^n = \mathcal{G}_{\leq d} \cap \mathcal{G}^k$ for all $k \geq n$, we can assume, without loss of generality, that $n \geq m$.

An element of $\mathcal{G}_d \cap \mathcal{G}^m \cap \mathcal{G}^{\mathrm{conn}}$ is called a *(organic) formula*. Hence a formula is an arrangement with degree requirement d. We call an isomorphism class of formulas a *compound* and every formula in it a *formula* of the compound. We write that a compound *has the formula* G to mean that G is a formula of the compound. A *sum of arrangements* respectively a *sum of formulas* is the sum of a finite set of arrangements respectively formulas with pairwise disjoint domains. Thus a sum of arrangements is an element of $\mathcal{G}_{\leq d} \cap \mathcal{G}^m$ and a sum of formulas an element of $\mathcal{G}_d \cap \mathcal{G}^m$.

Let $A_0, \ldots, A_k$ $(k \in \mathbb{N})$ be pairwise disjoint arrangements and $G = A_0 \oplus \ldots \oplus A_k$.

Proposition 12.1 $\{\mathrm{dom}(A_0), \ldots, \mathrm{dom}(A_k)\}$ *is the set of the components of* G.

Proof. Immediate consequence of Proposition 2.16. $\diamondsuit$

Proposition 12.2 *The sum* $A_0 \oplus \ldots \oplus A_k$ *is unique up to the order of the summands. (More precisely, if* $G = B_0 \oplus \ldots \oplus B_j$ *for pairwise disjoint arrangements* $B_0, \ldots, B_j$ $(j \in \mathbb{N})$*, then* $k = j$ *and* $\{A_0, \ldots, A_k\} = \{B_0, \ldots, B_j\}$*.)*

Proof. Immediate from the previous proposition. $\Diamond$

We call (precisely) each A_i $(0 \leq i \leq k)$ an *arrangement* of G and the compound C a *compound* of G iff some A_i $(0 \leq i \leq k)$ is a formula of C.

$a \in \mathrm{dom}(G)$ is called a *position* of G. A building symbol X *occurs* in G at a position a of G (a is a position *with* X in G, a is an X *position* of G) iff $s(\mathrm{val}_G(a, a)) = X$. A position with an atomic symbol in G is called an *atom* of G, a position with an implicit symbol is called *implicit* in G, a position with a $+$, $-$ respectively $\bullet$ is called a *positive charge*, a *negative charge* respectively an *electron* of G. A *charge* of G is a positive or negative charge of G. G is called *implicit* iff all its positions are implicit. It is called *atomic* iff it is not implicit.

Assume that b is a bond of multiplicity i and u, v are positions of G. b *joins* u to v in G iff $u \neq v$ are atoms of G and $R_i^G(u, v)$. u *carries* v in G iff $n \geq 1$, $u \neq v$, v is implicit in G and $R_1^G(u, v)$.

The reader attributing a chemical meaning to the definitions above should keep in mind that it does not really matter what formulas, like a $+$ position carrying a $+$ position or a $\bullet$ position, chemically mean. As we will see later, our concern are reactions and with an adequate choice of the starting compounds and of the reaction step notion such chemically rather weird constructions will not play any role. A $+$ position carrying a $-$ position, which form a “pair of opposite charges”, or two $\bullet$ positions carrying each other, which form a “bonding orbital”, could, on the other hand, be necessary for a proper chemical representation, as we will see later in the examples.

Proposition 12.3 *Every position of the sum G of arrangements is carried in G by at most one position and, if an implicit position p of G carries the position q in G, then q carries p in G.*

Proof. Exercise. $\diamondsuit$

We define

$G^\circ = B_0 \oplus \ldots \oplus B_j$, where $j \in \mathbb{N}$, $B_0, \ldots, B_j$ are pairwise distinct and $\{B_0, \ldots, B_j\}$ is the set of all atomic arrangements in $\{A_0, \ldots, A_k\}$, if G is atomic;

$G^\circ = \emptyset$, otherwise.

If H is a sum of arrangements, G, H are called *atomically equivalent* iff $G^\circ = H^\circ$.

A compound is called *implicit* respectively *atomic* if some (and thus every) formula of it is implicit respectively atomic. An *implicit*, *building* respectively *atomic symbol* of a compound is an implicit, building respectively atomic symbol occurring at a position of some (and thus every) formula of it.

Let now $A_0, \ldots, A_k$ ($k \in \mathbb{N}$) be pairwise non-isomorphic arrangements (i. e. $A_i \ncong A_j$ for $0 \leq i \neq j \leq k$) and $c\colon \{A_0, \ldots, A_k\} \to \mathbb{N}$. We denote by

$\sum_{A \in \{A_0, \ldots, A_k\}} c(A)A := c(A_0)A_0 + \ldots + c(A_k)A_k$

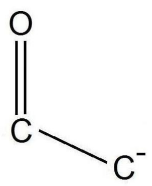
the class of all combinations of $\{A_0, \ldots, A_k\}$ with coefficients c.

Proposition 12.4 *The classes $c_0A_0 + \ldots + c_kA_k$ ($k \in \mathbb{N}, A_0, \ldots, A_k$ pairwise non-isomorphic arrangements, $c_0, \ldots, c_k \in \mathbb{N}$) are precisely the isomorphism classes of the sums of arrangements.*

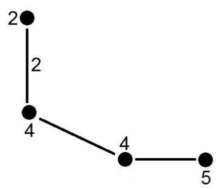
Proof. Straightforward from the definition. $\diamondsuit$

Throughout the examples in this chapter, we assume that $I = \{+, -, \bullet\}$, $n = 6$, $m = 2$, thus allowing only arrangements in which all bonds joining a position to another one are single or double, that the atomic symbols are **H**, **O**, **N**, **C**, their valence 1, 2, 3, 4 respectively and finally that s maps 0 to $+$, 1 to **H**, 2 to **O**, 3 to **N**, 4 to **C**, 5 to $-$ and 6 to $\bullet$. Consequently, we obtain $d = 1, 1, 2, 3, 4, 1, 1$.

The arrangement

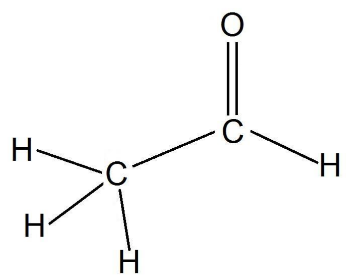


which is not a formula and in which a **C** position carries the $-$ position and a double bond joins a **C** to an **O** position, under the assumption of the proper identification of the positions, is the same as the arrangement depicted by

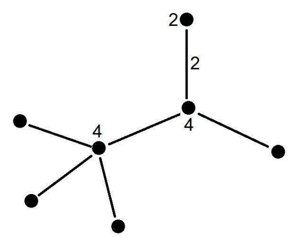


following the graphical representation of an n-multigraph in which the vertices are the elements of its domain and the valence in it is written on vertices and edges with the convention that the valence of a pair of distinct points between which there is no edge is 0 and the valence 1 is omitted on vertices and edges. We will also say that the two arrangements can be *identified* with each other.

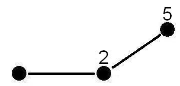
The formula



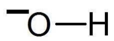
which in organic chemistry is recognized as a chemical formula of the organic compound acetaldehyde can be identified with the formula



Finally, the arrangement



can be identified with



and is known in chemistry as a chemical formula of the hydroxide ion.

A *semirule* is a pair (G, H) of sums of arrangements, the *left* and the *right side* of the semirule, that satisfies the *fundamental reaction principles*, i. e. the set of atoms of G is equal to the set of atoms of H and for all positions u of both G and H the building symbol occurring at u and the degree of u in G are the same as in H (i. e. $\mathrm{val}_G(u, u) = \mathrm{val}_H(u, u)$ and $\deg_G(u) = \deg_H(u)$). We denote the semirule (G, H) also by $G \to H$. Any compound of G is a *starting compound* and any compound of H a *product* of the semirule $G \to H$. A semirule where both sides are sums of formulas is called a *semiequation*. The semirules $G \to H$ and $K \to J$ are *atomically equivalent* iff G, K are atomically equivalent and H, J are atomically equivalent.

A semirule respectively a semiequation $G \to H$ for which G and H have the same positions (and hence are similar) is called a *reaction step rule*, or just a *rule* (not to be confused with an n-rule, defined in Section 3.1), respectively an *equation*. Obviously, if G is a sum of formulas and $G \to H$ a rule, then $G \to H$ is an equation. Indeed, if $G \to H$ is a rule, then for all canonical expansion $\bar{G}$ of G over $(\mathrm{S}_n)_r$ the pair $(\bar{G}, H)$ is an r-move for S_n.

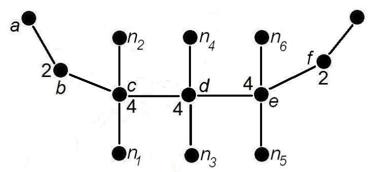
Let $G \to H$ be a semirule, $l_X(X \in I)$ be the number of X positions of G, that are carried by another position and are not a position of H and r_X the number of X positions of H, that are carried by another position and are not a position of G. It follows from graph theory that the sum of the degrees of the positions is even, whence that $\sum_{X \in I}(l_X - r_X)$ is even, which implies that $\sum_{X \in I} l_X$ and $\sum_{X \in I} r_X$ are both even or both odd. As a consequence every semirule respectively semiequation $G \to H$ is atomically equivalent to a rule respectively an equation.

Proposition 12.5 *To every rule $G \to H$ there is an injective $\mathcal{S}$-synthesis $K_0, \ldots, K_l$ with $K_0 = G$, $K_l = H$ and $\mathcal{S} \neq \emptyset$ the m-void set of n-rules. In particular there is an m-bound n-rule (G, u) with $H = \mathrm{sh}(G, u)$.*

Proof. Follows from Corollary 4.1 of the Shift Theorem. $\diamondsuit$

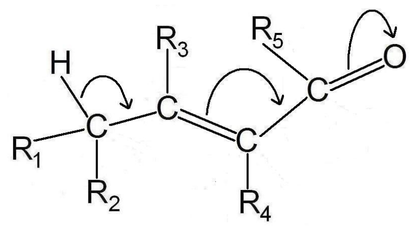
Let $\mathcal{R}$ be a set of rules. A sum H of arrangements is an *application* of $\mathcal{R}$ to a sum G of arrangements iff there is $K \to J \in \mathcal{R}$ such that the set $\{(\bar{K}, J)\}$ of the r-move $(\bar{K}, J)$ carries G into H for some (and thus for all) $r \in \mathbb{N}$ and canonical expansions $\bar{K}$ of K over $(\mathrm{S}_n)_r$. We abbreviate the notation by writing that H is an application of $K \to J$ to G iff it is an application of $\{K \to J\}$ to G.

$K \in \mathcal{G}_{\leq d} \cap \mathcal{G}^2$ can be identified with the 6-multigraph



and $u = a, b, c, d, a, d, e, f$. (8) is a 2-fold, separating elimination, since (K, u) is 2-fold, a 6-elimination and separating.

The last example, similar to the immediately previous one, is the set of semirules



(9)

($\mathrm{R}_1, \ldots, \mathrm{R}_5 = \mathbf{H}, \mathbf{C}$), known in organic chemistry as vinylogous enolization [3] [5], where the arrows are intended to put a negative charge on the symbol **O** and a positive charge on the symbol **H**. Let $\mathrm{R}_1, \ldots, \mathrm{R}_5 \in \{\mathbf{H}, \mathbf{C}\}$. Rule (9) is the pair $(K, \mathrm{sh}(K, u))$, where $K \in \mathcal{G}_{\leq d} \cap \mathcal{G}^2$ can be identified with the 6-multigraph

Proposition 12.7 *Let G be a formula of the compound C, H a sum of formulas and $\mathcal{A}$ the set of compounds of H. Assume that the valence of every building symbol is $\leq m$. Then C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}^{\mathcal{S}}$ iff every building symbol of C is a building symbol of a compound of $\mathcal{A}$.*

Proof. C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}^{\mathcal{S}}$ iff [with the definition of product and Corollary 12.1] G is a product of a combination of H iff [Corollary 4.3] for every position a of G there is a position b of H with $\mathrm{val}_G(a,a) = \mathrm{val}_H(b,b)$ iff every building symbol of C is a building symbol of a compound of $\mathcal{A}$. $\diamondsuit$

Proposition 12.7 implies that, if all implicit symbols of the compound C are implicit symbols of a compound in the set $\mathcal{A}$ of compounds, the criterion for synthesizability of C from $\mathcal{A}$ according to $\mathcal{R}^{\mathcal{S}}$ is the law of conservation of matter: C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}^{\mathcal{S}}$ iff every atomic symbol of C is also an atomic symbol of a compound of $\mathcal{A}$. The criterion for synthesizability according to the most general set of rules is the conservation of matter (which is also the most general principle of the chemical reactions).

12.1 Decidability results

From the statement that the criterion for synthesizability according to the most general set of rules is the conservation of matter we can immediately infer that a procedure exists which decides for a finite, m-void set $\mathcal{S}$ of n-rules, any compound C and any finite set $\mathcal{A}$ of compounds whether C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}^{\mathcal{S}}$.

The next decidability and undecidability results involve less general sets of rules.

Theorem 12.2 *There is a procedure that decides for any finite set $\mathcal{R}$ of basic additions, any compound C and any finite set $\mathcal{A}$ of compounds whether C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}$.*

Proof. Assume $\mathcal{A} \neq \emptyset$ is a finite set of compounds and that $\mathcal{R} = \mathcal{R}^{\mathcal{S}'}$, for a finite set $\mathcal{S}'$ of basic n-additions. Let G be a formula of the compound C, $\mathcal{F}$ a choice set of $\mathcal{A}$ with $\mathrm{dom}(K) \cap \mathrm{dom}(J) = \emptyset$ for all distinct formulas $K, J \in \mathcal{F}$. $\sum \mathcal{F}$ is a sum of formulas and, by setting $\mathcal{S}$ to be the set of all m-bound $P \in \mathcal{S}'$, we have $\mathcal{R} = \mathcal{R}^{\mathcal{S}}$. With Corollary 12.1 C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}$ iff C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}^{\mathcal{S}}$ iff [Corollary 12.1] G is an $\mathcal{S}$-product of a combination of $\mathcal{F}$ iff [Corollary 3.1] G is an $\mathcal{S}$-product of a combination of $\sum \mathcal{F}$. From Theorem 3.2 the basic addition problem is solvable. Now, the basic addition problem is solvable

iff the $\mathcal{R}^{\mathrm{ad}}$-synthesizability problem for $\mathcal{G}^{\mathrm{dr}}$ is solvable

iff the $\mathcal{R}^{\mathrm{ad}}$-synthesizability problem for $\mathcal{G}^{\mathrm{dr}}$, $\mathcal{G}$ is solvable

iff it is decidable given $n \in \mathbb{N}$, a set $\mathcal{S} \in \mathcal{R}^{\mathrm{ad}}$ of n-rules, n-multigraphs $H \in \mathcal{G}^{\mathrm{dr}}$ and $G \in \mathcal{G}$ whether G an $\mathcal{S}$-product of a combination of H

iff it is decidable given a set $\mathcal{S}$ of basic n-additions, $H, G \in \mathcal{G}^m \cap \mathcal{G}_d$ whether G an $\mathcal{S}$-product of a combination of H

iff it is decidable given a set $\mathcal{S}$ of basic n-additions, a sum H of formulas and a formula G whether G is an $\mathcal{S}$-product of a combination of H. $\diamondsuit$

The next proposition can be proven from Corollary 3.9 and Proposition 3.14 in a completely analogous way to the proof of Theorem 12.2.

Proposition 12.8 (a) *There is a procedure that decides for any finite set $\mathcal{R}$ of 1-fold, unfragmented and building rules, any compound C and any finite set $\mathcal{A}$ of compounds whether C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}$.*

(b) *There is a procedure that decides for any finite set $\mathcal{R}$ of separating rules, any compound C and any finite set $\mathcal{A}$ of compounds whether C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}$.* $\diamondsuit$

So, for example, there is a procedure that for any compound C and any finite set $\mathcal{A}$ of compounds decides whether C is synthesizable from $\mathcal{A}$ according to the set of rules that are rule (4) or in the set (8) of rules. With Corollary 3.8 we can state a stronger result than Proposition 12.8 (a):

If $\mathcal{R}$ is a set of 1-fold, unfragmented and building rules, then the compound C is syntesizable from the set $\mathcal{A}$ of compounds according to $\mathcal{R}$ iff there is a reaction according to $\mathcal{R}$ whose starting compounds are in $\mathcal{A}$ and whose right side is a formula of C.

The formal proof of this stronger result is completely straightforward and therefore a good exercise for the reader. The solution of the exercise is presented here:

Let $\mathcal{R}$ be a set of 1-fold, unfragmented and building rules, C a compound, $\mathcal{A}$ a set of compounds, G a formula of C and $\mathcal{F}$ a choice set of $\mathcal{A}$ whose elements have pairwise disjoint domains. $\mathcal{R} = \mathcal{R}^{\mathcal{S}}$ for a set $\mathcal{S}$ of 1-fold, unfragmented and building n-rules.

C is syntesizable from $\mathcal{A}$ according to $\mathcal{R}$

iff [Corollary 12.1] G is an $\mathcal{S}$-product of a combination of $\mathcal{F}$

iff [Corollary 3.1] G is an $\mathcal{S}$-product of a combination of $\sum \mathcal{F}$

iff [Proposition 3.5] G is a closed $\mathcal{S}$-product of a combination of $\sum \mathcal{F}$

iff [Corollary 3.8] G is $\mathcal{S}$-synthesizable from a combination of components of $\sum \mathcal{F}$

iff G is $\mathcal{S}$-synthesizable from a combination of $\mathcal{F}$

iff there is an $\mathcal{S}$-synthesis $H_0, \ldots, H_l$ with $H_l = G$ and H_0 a combination of $\mathcal{F}$

iff [Theorem 12.1] there is a synthesis $H_0, \ldots, H_{\bar{l}}$ according to $\mathcal{R}$ with $H_{\bar{l}} = G$ and H_0 a combination of $\mathcal{F}$

iff, because every compound of a combination of $\mathcal{F}$ is in $\mathcal{A}$, there is a reaction according to $\mathcal{R}$ whose starting compounds are in $\mathcal{A}$ and whose right side is a formula of C.

Once translated into the language built with the vocabulary of organic chemistry, which is an easy task, the proof of Proposition 3.14 delivers a procedure whose existence is claimed in Proposition 12.8 (b).

Assume now that $n = 14$, $m = 1$, the valence of $s(i)$ is 1 for $0 \leq i < 3$ and it is 2 for $3 \leq i \leq 14$. Let C be the compound whose formula is the 2-element $\mathrm{srp}_{14}(\emptyset)$ and $\mathcal{A}_0$ be the set of compounds of the sum of formulas H_0 to which Corollary 5.3 refers. Any formula of any compound in $\mathcal{A}_0$ has at most 6 positions. $\mathrm{arp}_{14}(\mathcal{T}_0) \neq \emptyset$ is a finite set of 2-fold 14-additions (K, u) with $|\mathrm{dom}(K)| \leq 12$. Corollary 5.3 and Corollary 12.1 imply the next proposition.

Theorem 12.3 *No procedure decides given a finite set $\mathcal{A}$ of compounds whether C is synthesizable from $\mathcal{A}$ according to $\mathcal{R}^{\mathrm{arp}_{14}(\mathcal{T}_0)}$ and no procedure decides given a compound D whether D is synthesizable from $\mathcal{A}_0$ according to $\mathcal{R}^{\mathrm{arp}_{14}(\mathcal{I}_0)}$.* $\diamondsuit$

12.2 Generalized set of rules

A *generalized set of rules* is an interpretation φ for S_n of arbitrary range r that carries any sum of arrangements at any r-sequence to its domain into a similar sum of arrangements.

Theorem 12.4 *For every finite set $\mathcal{R}$ of rules there is an m-bound, reactional interpretation φ for S_n and vice versa such that for all sums $G \neq H$ of arrangements H is an application of $\mathcal{R}$ to G iff φ carries G into H.*

Proof. Let $\mathcal{R}$ be a finite set of rules. Following Proposition 12.5 form a finite set $\mathcal{S}$ of m-bound n-rules such that $\mathcal{R}$ is the set of all $G \to \mathrm{sh}(G, u)$ with $(G, u) \in \mathcal{S}$. With Theorem 10.3 find an m-bound, reactional interpretation φ for S_n such that for all n-multigraphs G, H we have that H is an $\mathcal{S}$-shift of G iff φ carries G into H.

Because of Lemma 12.1 H is an $\mathcal{S}$-shift of G iff H is an application of $\mathcal{R}$ to G for all sums of arrangements $G \neq H$.

For the vice versa let φ be an m-bound, reactional interpretation φ for S_n. With Theorem 10.3 find a finite set $\mathcal{S}$ of finite m-bound n-rules such that H is an $\mathcal{S}$-shift of G iff φ carries G into H for all n-multigraphs G, H. Lemma 12.1 yields that for all sums $G \neq H$ of arrangements H is an $\mathcal{S}$-shift of G iff H is an application of $\mathcal{R}^{\mathcal{S}}$ to H. $\diamondsuit$

The association of an m-bound, reactional interpretation for S_n to a finite set $\mathcal{R}$ of rules goes one step further. It is often the case that we would like to have a notion of reaction that with every reaction $G \to H$ includes also its *reverse* $H \to G$. Therefore we define an equation $G \to H$ to be a *symmetrized reaction according* to $\mathcal{R}$ iff $G \to H$ or $H \to G$ is a reaction according to $\mathcal{R}$.

For a set A we define the *inverse* A' of A by $A' = \{(a, b)|(b, a) \in A\}$. A symmetrized reaction according to $\mathcal{R}$ is obviously a reaction according to $(\mathcal{R} \cup \mathcal{R}')$ and $(\mathcal{R} \cup \mathcal{R}')' = (\mathcal{R} \cup \mathcal{R}')$. $(\mathcal{R} \cup \mathcal{R}')$ is therefore invariant under inversion.

It is now a consequence of the next proposition that for every finite set $\mathcal{R}$ of rules there is an m-bound, reactional interpretation φ for S_n, which maintains the invariance under inversion (i. e. with $\varphi' = \varphi$), such that for all sums $G \neq H$ of arrangements $G \to H$ is a symmetrized reaction according to $\mathcal{R}$ iff H is φ-derivable from G.

Proposition 12.9 *For every finite set $\mathcal{R}$ of rules there is an m-bound, reactional interpretation φ for S_n, satisfying $\varphi' = \varphi$, such that for all sums $G \neq H$ of arrangements H is an application of $(\mathcal{R} \cup \mathcal{R}')$ to G iff φ carries G into H.*

Proof. By Theorem 12.4 there is an m-bound, reactional interpretation φ for S_n such that for all sums $G \neq H$ of arrangements H is an application of $(\mathcal{R} \cup \mathcal{R}')$ to G iff φ carries G into H. By Proposition 10.22 there is a reactional interpretation ψ for S_n, satisfying $\psi' = \psi$, that, for all n-multigraphs G, H, carries G into H iff φ carries G into H or H into G. But for all sums $G \neq H$ of arrangements φ carries G into H iff it carries

H into G, whence ψ is a reactional interpretation for S_n such that for all sums $G \neq H$ of arrangements H is an application of $(\mathcal{R} \cup \mathcal{R}')$ to G iff ψ carries G into H. ψ is, indeed, m-bound. $\diamondsuit$

Because of Theorem 12.4 and Proposition 12.9 it is natural to increase the expressive power of the finite sets of rules by allowing a generalized set of rules φ to be used in place of a finite set of rules, more specifically, by defining, first of all, that, for the sums G, H of arrangements, H is an application of φ to G iff φ carries G into H and, subsequently, corresponding to the definitions according to a set of rules, by defining *synthesis*, *synthesis from* a set of compounds, *synthesis of* a compound, *synthesizable (in l steps)* from a set of compounds, *(l-step) reaction* and *reaction step*, all, of course, according to φ.

Till the end of this chapter let $\mathcal{A}$ be a set of compounds, the set $\mathcal{F}$ of formulas a choice set of $\mathcal{A}$, δ a sentence in S_n and φ a generalized set of rules of range r.

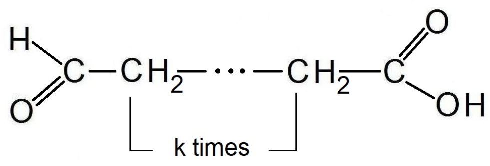
Another generalization similar to the one regarding the set of rules allows first-order sentences to be synthesizable according to φ from a set of compounds: δ is *synthesizable (in l steps) according to φ* from $\mathcal{A}$ iff there is a (l-step) reaction according to φ whose right side satisfies δ and whose starting compounds belong all to $\mathcal{A}$.

Proposition 12.10 *δ is synthesizable in l steps according to φ from $\mathcal{A}$ iff δ is φ-derivable in l steps from a finite combination of $\mathcal{F}$.*

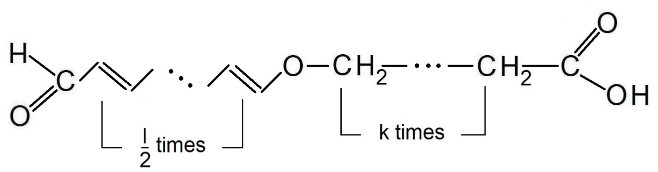
Proof. δ is synthesizable in l steps according to φ from $\mathcal{A}$ iff there is a synthesis $G_0, \ldots, G_l$

As we did in Section 7.3 with Theorem 7.7 we look at some examples of Proposition 12.12, that are built on the examples in Section 7.3, which used k- and $\langle l, k\rangle$-paths.

We refer back to the initial settings of I, n, m, the valence, the functions s, d and to the graphical representation of n-multigraphs. Let F_k ($k \in \mathbb{N}$) be the formula



and $F_{l,k}$ ($k, l \in \mathbb{N}$, l even) the formula



and E the formula $+ \, -$. We set

$\mathcal{F}_k = \{F_j \,|\, 0 \le j \le k\} \cup \{E\}$;

$\mathcal{D} = \{F_k \,|\, k \in \mathbb{N}\} \cup \{E\}$;

$\mathcal{A}$ equal to the set of all compounds with a formula in $\mathcal{D}$;

$\mathcal{A}_k$ equal to the set of all compounds with a formula in $\mathcal{F}_k$;

$\mathcal{F}_{l,k} = \{F_{i,j} \,|\, 0 \le i \le l, i \text{ even and } 0 \le j \le k\} \cup \{E\}$;

$\mathcal{E} = \{F_{l,k} \mid l, k \in \mathbb{N} \text{ and } l \text{ even}\} \cup \{E\}$;

$\mathcal{B}$ equal to the set of all compounds with a formula in $\mathcal{E}$;

$\mathcal{B}_{l,k}$ equal to the set of all compounds with a formula in $\mathcal{F}_{l,k}$;

$\mathcal{G} = \{F_{36,52}, F_{36,51}, F_{34,52}, F_{34,51}, F_{16,51}, F_{16,52}, F_{16,53}, F_{16,54}\}$;

$\mathcal{C}$ equal to the set of all compounds with a formula in $\mathcal{G}$.

It requires a moment of thought to verify that for all $r, m, l_0, l_1, k_0, k_1 \in \mathbb{N}$

(a) if the k_0-path is $2, r, m$-equivalent to the k_1-path, then $F_{k_0} \equiv_{2,r,m} F_{k_1}$;

(b) if the alternate l_0-path is $2, r, m$-equivalent to the alternate l_1-path and the k_0-path $2, r, m$-equivalent to the k_1-path, then $F_{l_0,k_0} \equiv_{2,r,m} F_{l_1,k_1}$.

Let $i, l \in \mathbb{N}$, $i \neq 0$, $l \geq 2$ and define $(h_j)_{1 \leq j \leq 2i+l}$, $(\bar{h}_j)_{1 \leq j \leq 2i+l}$ after the definition in Section 7.3, by putting $m = l$, $n = 2$ and therefore $r = 4$.

Because of (a) and Theorem 6.2, the $2i + l$-sequence Q, where Q_j is the equivalence relation over the class of all formulas isomorphic to a formula in $\mathcal{D}$ (i. e. of the type F_k for some $k \in \mathbb{N}$) such that $\cong$ is finer than Q_j and for all $k_0, k_1 \in \mathbb{N}$

$$Q_j(F_{k_0}, F_{k_1}) \text{ iff } k_0 = k_1 \text{ or } k_0, k_1 \geq h_{j+1}$$

$(0 \leq j \leq 2i + l)$, is a $[2, 4i, l]$-sequence over $\mathcal{D}$.

Because of (b), Theorem 6.2 and Proposition 6.21, the $2i + l$-sequence P, where P_j is the equivalence relation over the class of all formulas isomorphic to a formula in $\mathcal{E}$

such that $\cong$ is finer than P_j and for all $l_0, l_1, k_0, k_1 \in \mathbb{N}$ with l_0, l_1 even

$$P_j(F_{l_0,k_0}, F_{l_1,k_1}) \text{ iff } l_0 = l_1 \text{ or } l_0, l_1 \geq \bar{h}_{j+1} \quad \text{and} \quad k_0 = k_1 \text{ or } k_0, k_1 \geq h_{j+1}$$

$(0 \leq j \leq 2i + l)$, is a $[2, 4i, l]$-sequence over $\mathcal{E}$, whence over $\mathcal{G}$.

$\beta\colon \mathcal{D} \to \mathbb{N}$ with

$\beta(F_k) = \alpha(U_k)\ (k \in \mathbb{N}),\ \beta(E) = 2i + l,$

where α is given by (1) of Section 7.3, is a Q-combination function over $\mathcal{D}$ and $\mathcal{F}_{h_1}$ a choice set of $\mathcal{D}/Q_0$.

$\gamma\colon \mathcal{E} \to \mathbb{N}$ with

$\gamma(F_{l,k}) = \alpha(U_{l,k})\ (l, k \in \mathbb{N},\ l \text{ even}),\ \gamma(E) = 2i + l,$

where α is given by (3) of Section 7.3, is a P-combination function over $\mathcal{E}$ and $\mathcal{F}_{\bar{h}_1,h_1}$ a choice set of $\mathcal{E}/P_0$.

Let $\zeta(x_0, x_1, x_2, x_3)$ be a first-order formula in S_6, in which x_3 occurs free, and the interpretation φ for S_6 of range 4 be constructed from ζ as at the beginning of Section 10.1. $\mathrm{qr}(\varphi) = \mathrm{qr}(\zeta)$. By Lemma 10.1

$$\zeta\text{-shift}(G, u) = \varphi(G, u)$$

for all 6-multigraphs G and 4-sequences u to $\mathrm{dom}(G)$. φ is a connected modulo 2 generalized set of rules. Let $l = i\mathrm{qr}(\zeta) + l_0$ with $l_0 \geq 2$. We begin with examining the synthesizability from $\mathcal{A}$. Abbreviate

$$M = 1 + \sum_{j=1}^{2i+l} h_j = (2^l + 2) \sum_{j=1}^{2i} (2i)/j \ +\ 2^{l+1}(i+1) - 2(i+1).$$

The next proposition follows from Proposition 12.12.

Proposition 12.13 *A first-order property π expressible in* S_6 *with quantifier rank* l_0 *is synthesizable in $\leq i$ steps according to φ from $\mathcal{A}$ iff there is a $\leq i$-step reaction $G \to H$ according to φ for which H has π and G is of the type $\sum_{j=0}^{h_1} c_j F_j \ + \ dE$ with $c_j \leq \beta(F_j)$ $(0 \leq j \leq h_1)$ and $d \leq 2i + l$ iff there is a $\leq i$-step reaction according to φ whose right side has π and whose left side is of the type $\sum_{j=0}^{h_1} c_j F_j \ + \ dE$, where $\sum_{j=0}^{h_1} c_j \leq M$, $c_j \leq 2i + l$ $(0 \leq j \leq h_1)$ and $d \leq 2i + l$.* ♢

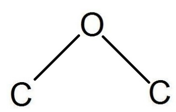
The synthesizability from $\mathcal{B}$ is handled similarly to the synthesizability from $\mathcal{A}$. Abbreviate

$$M = (\frac{\bar{h}_1}{2} + 1)(h_1 + 1) + \sum_{j=2}^{2i+l} \frac{\bar{h}_j}{2} h_j = \sum_{j=1}^{2i} \frac{\bar{h}_j}{2} h_j \ + \ \sum_{j=1}^{l-1} 2^{2(l-j)+1} \ + \ \frac{\bar{h}_1}{2} + h_1 + 2.$$

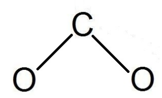
Again the next proposition follows from Proposition 12.12.

Proposition 12.14 *A first-order property π expressible in* S_6 *with quantifier rank* l_0 *is synthesizable in $\leq i$ steps according to φ from $\mathcal{B}$ iff there is a $\leq i$-step reaction $G \to H$ according to φ for which H has π and G is of the type $\sum_{l=0}^{\bar{h}_1} \sum_{k=0}^{h_1} c_{l,k} F_{l,k} \ + \ dE$ with $c(l,k) \leq \gamma(F_{l,k})$ $(0 \leq l \leq \bar{h}_1,\ 0 \leq k \leq h_1,\ l$ even$)$ and $d \leq 2i + l$ iff there is a $\leq i$-step reaction according to φ whose right side has π and whose left side is of the type $\sum_{l=0}^{\bar{h}_1} \sum_{k=0}^{h_1} c_{l,k} F_{l,k} \ + \ dE$, where $\sum_{l=0}^{\bar{h}_1} \sum_{k=0}^{h_1} c_{l,k} \leq M$, $c_{l,k} \leq 2i + l$ $(0 \leq l \leq \bar{h}_1,\ 0 \leq k \leq h_1,\ l$ even$)$ and $d \leq 2i + l$.* ♢

To make a numerical example of Proposition 12.13 with a concrete first order property, we set $i = 4, \mathrm{qr}(\zeta) = 1, l_0 = 2$ and add two definitions. We call a compound an *ether* iff it has a formula containing the arrangement



We call a compound an *acetal* iff it has a formula containing the arrangement

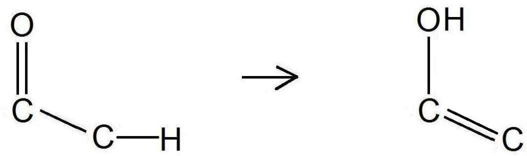


The property of a sum of formulas that one of its compounds is an ether but none an acetal is first-order expressible with quantifier rank 2. Therefore we can state that there is a $\leq$ 4-step reaction according to φ whose starting compounds are in $\mathcal{A}$ with a product that is an ether and no products that are acetals iff there is a $\leq$ 4-step reaction according to φ whose left side is of the type

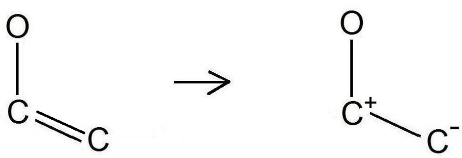
$$\sum_{j=327}^{591} c_j^1 F_j + \sum_{j=195}^{326} c_j^2 F_j + \sum_{j=129}^{194} c_j^4 F_j + \sum_{j=64}^{128} c_j^8 F_j + \sum_{j=32}^{63} c_j^9 F_j + \sum_{j=16}^{31} c_j^{10} F_j + \sum_{j=8}^{15} c_j^{11} F_j + \sum_{j=4}^{7} c_j^{12} F_j + \sum_{j=1}^{3} c_j^{13} F_j + c_1^{14} F_0 + c_2^{14} E$$

with each $c_j^k \leq k$, having a product that is an ether and no products that are acetals.

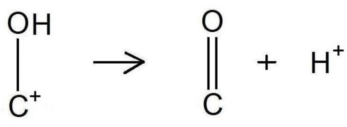
For this example we used the sequence $(h_j)_{0\leq j\leq 14}$ that has been calculated in Section 7.3. Regarding the generalized set of rules φ with $\mathrm{qr}(\varphi) = 1$, it should be remarked that the set of rules (2) and (3), previously listed, can be easily expressed as a ζ-shift for some first-order formula $\zeta(x_0, x_1, x_2, x_3)$ in S_6 (in which x_3 occurs free) with $\mathrm{qr}(\zeta) = 1$. Rule (1), however, can not, but it can be replaced by the following, admittetly a little less strong, rules, which can be expressed as a ζ-shift for some ζ as above.



(10)



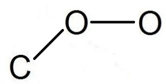
(11)



(12)

Therefore the set of rules (2), (3), (10), (11) and (12) is a very simple instance of the generalized set of rules φ we are considering in this example.

To make a numerical example of Proposition 12.14 with a concrete first order property, we set $i = 3, \mathrm{qr}(\zeta) = 1, l_0 = 2$ and add one more definition. We call a compound a *peroxide* iff it has a formula containing the arrangement



The property of a sum of formulas that one of its compounds is a peroxide but none an acetal is first-order expressible with quantifier rank 2. Therefore we can state that there is a $\leq$ 3-step reaction according to φ whose starting compounds are in $\mathcal{B}$ with a product that is a peroxide and no products that are acetals iff there is a $\leq$ 3-step reaction according to φ whose left side is of the type

$$\sum_{l=68}^{120} \sum_{k=0}^{235} c^1_{2l,k} F_{2l,k} + \sum_{l=0}^{67} \sum_{k=133}^{235} c^1_{2l,k} F_{2l,k} + \sum_{l=50}^{67} \sum_{k=0}^{132} c^2_{2l,k} F_{2l,k} +$$
$$\sum_{l=0}^{49} \sum_{k=99}^{132} c^2_{2l,k} F_{2l,k} + \sum_{l=33}^{49} \sum_{k=0}^{98} c^3_{2l,k} F_{2l,k} + \sum_{l=0}^{32} \sum_{k=65}^{98} c^3_{2l,k} F_{2l,k} +$$
$$\sum_{l=16}^{32} \sum_{k=0}^{64} c^6_{2l,k} F_{2l,k} + \sum_{l=0}^{15} \sum_{k=32}^{64} c^6_{2l,k} F_{2l,k} + \sum_{l=8}^{15} \sum_{k=0}^{31} c^7_{2l,k} F_{2l,k} +$$
$$\sum_{l=0}^{7} \sum_{k=16}^{31} c^7_{2l,k} F_{2l,k} + \sum_{l=4}^{7} \sum_{k=0}^{15} c^8_{2l,k} F_{2l,k} + \sum_{l=0}^{3} \sum_{k=8}^{15} c^8_{2l,k} F_{2l,k} +$$
$$\sum_{l=2}^{3} \sum_{k=0}^{7} c^9_{2l,k} F_{2l,k} + \sum_{l=0}^{1} \sum_{k=4}^{7} c^9_{2l,k} F_{2l,k} + \sum_{l=1}^{1} \sum_{k=0}^{3} c^{10}_{2l,k} F_{2l,k} +$$
$$\sum_{l=0}^{0} \sum_{k=1}^{3} c^{10}_{2l,k} F_{2l,k} + c^{11}_1 F_{0,0} + c^{11}_2 E.$$

with each $c^j_{2l,k} \leq j$ and $c^{11}_1, c^{11}_2 \leq 11$, having a product that is a peroxide and no products that are acetals. For this example we used the sequence $(\bar{h}_j)_{0 \leq j \leq 11}$, $(h_j)_{0 \leq j \leq 11}$ that have been already calculated in Section 7.3.

To make a third numerical example, this time using the set $\mathcal{G}$, we set $i = 2$, $\mathrm{qr}(\zeta) = 1$, $l_0 = 2$. Then D is a $[2, 8, 4]$-sequence over $\mathcal{G}$. From the third example in Section 7.3, in which the sequence Q has been defined by

$$Q = \equiv_{2,8,4}, \equiv_{2,4,4}, \equiv_{2,2,4}, \equiv_{2,2,4}, \equiv_4, \equiv_3, \equiv_2, \equiv_1,$$

we infer that $D_j(F_{l_0,k_0}, F_{l_1,k_1})$ iff $Q_j(U_{l_0,k_0}, U_{l_1,k_1})(F_{l_0,k_0}, F_{l_1,k_1} \in \mathcal{G},\ 0 \leq j \leq 8)$. Therefore $(1)_{G \in \mathcal{G}}$ is a D-combination function over $\mathcal{G}$ and $\mathcal{G}$ a choice set of $\mathcal{G}/D_0$. This allows us, for example, the conclusion that there is a 0-, 1- or 2-step reaction according to φ whose left side, for some $c_0, \ldots, c_7 \in \mathbb{N}$ is of the type

$$c_0 F_{36,52} + c_1 F_{36,51} + c_2 F_{34,52} + c_3 F_{34,51} + c_4 F_{16,51} + c_5 F_{16,52} + c_6 F_{16,53} + c_7 F_{16,54}$$

with a product that is a peroxide and no products that are acetals iff there is a 0-, 1- or 2-step reaction according to φ with a product that is a peroxide and no products that are acetals, whose left side is of the type

$$c_0 F_{36,52} + c_1 F_{36,51} + c_2 F_{34,52} + c_3 F_{34,51} + c_4 F_{16,51} + c_5 F_{16,52} + c_6 F_{16,53} + c_7 F_{16,54},$$

where every c_j $(0 \leq j \leq 7)$ is 0 or 1.

In the following, last part of this section we apply some of the results obtained in Chapter 9 to the synthesizability according to φ from $\mathcal{A}$. In order to do this, we assume that $\mathcal{A}$ is finite and φ weakly invertible.

Let $\mathcal{G}$ be the class of all sums of formulas whose compounds are in $\mathcal{A}$ and $\mathcal{C}$ be the class of all right sides of a reaction according to φ whose starting compounds are in $\mathcal{A}$. We will find a few conditions for the existence of a procedure that decides for all sentences in S_n whether they are synthesizable according to φ from $\mathcal{A}$, as well as for the axiomatizability of $\mathcal{C}$ in the finite.

First of all, we notice that $\mathcal{G} = \mathrm{cmb}(\mathcal{F})^{\mathrm{f}}$, $\mathcal{C} = \vec{\varphi}(\mathcal{G}) = (\vec{\varphi}(\mathrm{cmb}(\mathcal{F})))^{\mathrm{f}}$ and that $\mathcal{F}$, being a choice set of $\mathcal{A}$, is a finite set of pairwise non-isomorphic, connected, m-bound n-multigraphs with degree requirement d. m, n, d have been set, once for this whole chapter, at the beginning of it. The sentence $\vartheta_{\mathcal{F}}$ was defined in Section 2.5 and satisfies $\mathrm{cmb}(\mathcal{F}) = \mathrm{mod}^{\mathrm{S}_n}(\vartheta_{\mathcal{F}})$. Set $\xi_j = \exists c_0 \dots c_{rj-1} \vartheta_{\mathcal{F}} \varphi'^j$.

Theorem 12.5 *The following statements are equivalent for all $i \in \mathbb{N}$:*

(i) *i is the least $k \in \mathbb{N}$ such that every sentence in S_n that is synthesizable according to φ from $\mathcal{A}$ is synthesizable in $\leq k$ steps according to φ from $\mathcal{A}$.*

(ii) *i is the least elementary bound of $\mathcal{G}, \varphi$.*

(iii) *i is the least $k \in \mathbb{N}$ for which $(\bigvee_{j \in \mathbb{N}} \xi_j \leftrightarrow \bigvee_{0 \leq j \leq k} \xi_j)$ holds in all finite structures over S_n.*

(iv) *The rank of $\mathcal{G}, \varphi$ is i.*

(v) *The rank of $\mathrm{cmb}(\mathcal{F}), \varphi$ is i.*

(vi) *i is the least $k \in \mathbb{N}$ with* $\models (\bigvee_{j\in\mathbb{N}} \xi_j \leftrightarrow \bigvee_{0\le j\le k} \xi_j)$.

(vii) *i is the least elementary bound of* $\mathrm{cmb}(\mathcal{F}), \varphi$.

Proof. (i) $\Leftrightarrow$ (ii) follows directly from Corollary 12.2 and the definition of elementary bound. The pairwise equivalence of (ii) - (vii) is an immediate consequence of Theorem 9.6. $\diamondsuit$

Theorem 12.6 *The following statements are equivalent:*

(i) *There is $i \in \mathbb{N}$ such that every sentence in S_n that is synthesizable according to φ from $\mathcal{A}$ is synthesizable in $\le i$ steps according to φ from $\mathcal{A}$.*

(ii) $\vec{\varphi}(\mathrm{cmb}(\mathcal{F}))$ *is axiomatizable.*

(iii) $\vec{\varphi}(\mathrm{cmb}(\mathcal{F}))$ *is closed under ultraproducts.*

(iv) $\bigvee_{0\le j\le i} \xi_j$ *axiomatizes* $\vec{\varphi}(\mathrm{cmb}(\mathcal{F}))$ *for some $i \in \mathbb{N}$.*

(v) *The rank of* $\mathrm{cmb}(\mathcal{F}), \varphi$ *is not ∞.*

(vi) *There is an elementary bound of* $\mathrm{cmb}(\mathcal{F}), \varphi$.

(vii) *There is an elementary bound of $\mathcal{G}, \varphi$.*

(viii) *The rank of $\mathcal{G}, \varphi$ is not ∞.*

(ix) $\bigvee_{0\le j\le i} \xi_j$ *axiomatizes $\mathcal{C}$ in the finite for some $i \in \mathbb{N}$.*

Proof. (i) $\Leftrightarrow$ (vi) follows from Theorem 12.5. The pairwise equivalence of (ii) - (ix) is an instance of Theorem 9.7. $\diamondsuit$

Proposition 12.15 *Assume that one (and thus all) of* (i) - (ix) *in Theorem* 12.6 *holds.*

(a) *There is a procedure that decides for all sentences in* S_n *whether they are synthesizable according to* φ *from* $\mathcal{A}$.

(b) $\mathrm{Th}(\vec{\varphi}(\mathrm{cmb}(\mathcal{F})))$ *is decidable.*

(c) $\mathrm{Th}(\mathcal{C})$ *is decidable.*

Proof. Corollary 9.8 states that the φ-derivability problem for $\mathrm{cmb}(\mathcal{F})$ is solvable. Now, Proposition 12.11 yields (a). (b) is an instance of Corollary 9.9. (c) follows from Corollary 7.24 and (b), given that $\mathcal{C} = (\vec{\varphi}(\mathrm{cmb}(\mathcal{F})))^{\mathrm{f}}$. $\diamondsuit$

Assume that φ is quantifier-free, which is in particular the case if it is m-bound and reactional. Proposition 9.4 yields:

Proposition 12.16 *Assume that one (and thus all) of* (i) - (ix) *in Theorem* 12.6 *holds.*

(a) $\vec{\varphi}(\mathrm{cmb}(\mathcal{F}))$ *is axiomatized by a sentence in* Σ_3^{L}.

(b) $\vec{\varphi}(\mathrm{cmb}(\mathcal{F}))$ *is preserved under 3-fillings.* $\diamondsuit$

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[2] H. Kaufmann, A. Häderer, *Grundlagen der organischen Chemie*, Birkhäuser Verlag, Basel Boston Berlin, 10. Auflage, 1996, p. 123.

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List of Abbreviations

$\mathbb{N}$ set of natural numbers, page 28

$\in, \subseteq$ element, subset relation, page 28

$\emptyset$ emptyset, page 28

$\cup, \bigcup$ union of sets, page 28

$\cap, \bigcap$ intersection of sets, page 28

$A \setminus B$ complement of B in A, page 28

A^n n-fold cartesian product of A, page 28

$|A|$ cardinality of A, page 28

$\mathrm{dom}(f)$, $\mathrm{rg}(f)$ domain, range of the function f, page 28

id_A identity function on A, page 28

$f \circ g$ composition of the functions f, g, page 28

p, q concatenation of the sequences p, q, page 29

$\wedge, \vee, \neg, \forall, \exists, \bigwedge, \bigvee$ logical symbols, page 29

$f\colon A \to B$ f is a function from A to B, page 30

ν_F arity of the symbol F, page 29

$\varphi(x_0, \dots, x_{k-1})$ variables free in φ, page 29

$\varphi[\,]$ substitution in φ, page 29

$\mathrm{qr}(\varphi)$ quantifier rank of φ, page 29

$\mathrm{dom}(U)$ domain of the structure U, page 30

R^U interpretation of the relation symbol R in the structure U, page 30

f^U interpretation of the function symbol f in the structure U, page 30

c^U interpretation of the constant c in the structure U, page 30

$U \restriction \mathrm{L}$ reduct of the structure U to L, page 30

(U, A) expansion of U with the elements of A, page 30

$U, (S{:}F)$ expansion of U with S, page 30

$\cong$ isomorphic, page 31

$\subseteq, \supseteq$ substructure, extension, page 31

$U|A$ restriction of the structure U to the set A, page 31

$U|A$ restriction of the structure U with constants to the set A, page 115

$e_{U,V}$ unique homomorphism from canonical U to V, page 31

$\sum \mathcal{U}$ sum of the set $\mathcal{U}$ of structures, page 31

Π_i^{S}, Σ_i^{S} prefix based sets of formulas in S, page 36

A/Q set of equivalence classes of A by Q, page 36

$\alpha_{E,\mathcal{U}}^{\mathcal{V}}$, page 37

S_n n-multigraph symbols, page 43

T_n n-multigraph theory, page 43

$\mathrm{val}_G()$ valence in G, page 43

$\deg_G()$ degree in G, page 44

$\mathrm{nb}_G()$ neighbourhood in G, page 47

$\mathrm{nb}_G^k()$ k-neighbourhood in G, page 48

$\mathrm{nb}_U^k()$ k-neighbourhood in the structure U, page 116

$\mathrm{cl}_G()$ closure in G, page 48

$\mathrm{gf}(U)$ Gaifman graph of U with constants, page 116

$\mathrm{gf}(U)$ Gaifman graph of U, page 54

$\deg_U()$ degree in the structure U, page 54

$\vartheta_{\mathcal{U}}$ axiom for the combinations of $\mathcal{U}$, page 61

$\tilde{u}$ sequence for the inverse shift, page 65

$\mathrm{sh}(G, u)$ shift of G at u, page 64

$\mathrm{sh}^{-1}(G, u)$ inverse shift of G at u, page 65

$\mathcal{S}$-$\mathrm{sh}(G, u)$ $\mathcal{S}$-shift of G at u, page 66

ζ-$\mathrm{sh}(G, u)$ ζ-shift of G at u, page 73

$\mathcal{G}$ class of all finite n-multigraphs, page 74

$\mathcal{R}$ class of all finite sets of finite n-rules, page 74

$\mathcal{G}_d$ class of all finite n-multigraphs with degree requirement d, page 75

$\mathcal{G}^m$ class of all finite, m-bound n-multigraphs, page 75

$\mathcal{G}^{\mathrm{xy}}$ subclass of $\mathcal{G}$ with some property, page 75

$\mathcal{R}^{\mathrm{xy}}$ subclass of $\mathcal{R}$ with some property, page 75

d_n a degree requirement function, page 76

$\tilde{\mathrm{S}}_n$ $\{R_4, \ldots, R_n\}$, page 101

$\mathrm{nrp}_n()$ natural n-representation, page 104

$\mathrm{srp}_n()$ second n-representation, page 104

$\mathrm{trp}_n()$ third n-representation, page 104

$\mathrm{arp}_n()$ addition n-representation, page 106

C_0^U set of values in U of the constants in C_0, page 115

$U^k(A)$ restriction of U to its k-neighbourhood of A and the constants, page 116

$\mathrm{lft}(U)$, $\mathrm{rgt}(U)$ left, right end point of an r, k-path, page 123

$\mathrm{ctr}(U)$ element with S in an $r, \langle l, k\rangle$-path, page 140

L_r $L \cup \{c_0, \ldots, c_{r-1}\}$, page 147

(U, u) expansion of U with u for $c_0, \ldots, c_{r-1}$, page 147

ω^L identity interpretation, page 147

$\mathrm{qr}(\varphi)$ quantifier rank of the interpretation φ, page 147

$\varphi(U)$ structure φ defines in U, page 148

$\leftrightarrow$ equivalence between interpretations, page 148

$\varphi|\gamma$ φ relativised by γ, page 149

$\mathrm{dom}(\varphi)$ domain of the interpretation φ, page 150

ζ_φ axiom for $\mathrm{dom}(\varphi)$, page 150

E^φ function induced by φ, page 158

Φ^F interpretation associated to F, page 159

$\varphi^i(\mathcal{C})$ class of structures φ-derivable in i steps from $\mathcal{C}$, page 153

$\varphi^{\leq i}(\mathcal{C})$ class of structures φ-derivable in $\leq i$ steps from $\mathcal{C}$, page 153

$\vec{\varphi}(\mathcal{C})$ class of structures φ-derivable from $\mathcal{C}$, page 153

$\psi\,\varphi$ composition of ψ, φ, page 165

φ^n n-th power of the interpretation φ, page 167

n/m integer quotient of n and m, page 171

$|\mathcal{U}|_E$, page 177

φ' inverse interpretation, page 190

$\Rightarrow_\Sigma$ relation between structures based on Σ, page 201

$\mathcal{M}^\varphi$ set of r-moves for φ, page 242

$\Psi^\mathcal{R}$ interpretation for the replacement $\mathcal{R}$, page 244

G° sum of atomic arrangements, page 275

Index