Logical Equivalences, Homomorphism Indistinguishability, and Forbidden Minors

Tim Seppelt
RWTH Aachen University, Germany

Abstract

Two graphs G and H are *homomorphism indistinguishable* over a class of graphs $\mathcal{F}$ if for all graphs $F \in \mathcal{F}$ the number of homomorphisms from F to G is equal to the number of homomorphisms from F to H. Many natural equivalence relations comparing graphs such as (quantum) isomorphism, spectral, and logical equivalences can be characterised as homomorphism indistinguishability relations over certain graph classes.

Abstracting from the wealth of such instances, we show in this paper that equivalences w.r.t. any *self-complementarity* logic admitting a characterisation as homomorphism indistinguishability relation can be characterised by homomorphism indistinguishability over a minor-closed graph class. Self-complementarity is a mild property satisfied by most well-studied logics. This result follows from a correspondence between closure properties of a graph class and preservation properties of its homomorphism indistinguishability relation.

Furthermore, we classify all graph classes which are in a sense finite (*essentially profinite*) and satisfy the maximality condition of being *homomorphism distinguishing closed*, i.e. adding any graph to the class strictly refines its homomorphism indistinguishability relation. Thereby, we answer various questions raised by Roberson (2022) on general properties of the homomorphism distinguishing closure.

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1 Introduction

In 1967, Lovász [23] proved that two graphs G and H are isomorphic if and only if they are *homomorphism indistinguishable* over all graphs, i.e. for every graph F, the number of homomorphisms from F to G is equal to the number of homomorphisms from F to H. Since then, homomorphism indistinguishability over restricted graph classes has emerged as a powerful framework for capturing a wide range of equivalence relations comparing graphs. For example, two graphs have cospectral adjacency matrices iff they are homomorphism indistinguishable over all cycles, cf. [13]. They are quantum isomorphic iff they are homomorphism indistinguishable over all planar graphs [25].

Most notably, equivalences with respect to many logic fragments can be characterised as homomorphism indistinguishability relations over certain graph classes [19, 12, 27, 31]. For example, two graphs satisfy the same sentences of k-variable counting logic iff they are homomorphism indistinguishable over graphs of treewidth less than k [14]. All graph classes

Table 1 Overview of results on equivalent properties of a homomorphism distinguishing closed graph class $\mathcal{F}$ and of its homomorphism indistinguishability relation $\equiv_{\mathcal{F}}$.

Closure property of $\mathcal{F}$	Preservation property of $\equiv_{\mathcal{F}}$	Theorem
taking minors	complements	Theorem 9
taking summands	disjoint unions	Theorem 5
taking subgraphs	full complements	Theorem 6
taking induced subgraphs	left lexicographic products	Theorem 12
contracting edges	right lexicographic products	Theorem 13

featured in such characterisations are minor-closed and hence of a particularly enjoyable structure. The main result of this paper asserts that this is not a mere coincidence: In fact, logical equivalences and homomorphism indistinguishability over minor-closed graph classes are intimately related.

To make this statement precise, the term "logic" has to be formalised. Following [15], a *logic on graphs* is a pair $(\mathsf{L}, \models)$ of a class L of *sentences* and an isomorphism-invariant[1] *model relation* $\models$ between graphs and sentences. Two graphs G and H are L-*equivalent* if $G \models \varphi$ iff $H \models \varphi$ for all $\varphi \in \mathsf{L}$. One may think of a logic on graphs as a collection of isomorphism-invariant graph properties. A logic is called *self-complementary* if for every $\varphi \in \mathsf{L}$ there is an element $\overline{\varphi} \in \mathsf{L}$ such that $G \models \varphi$ if and only if $\overline{G} \models \overline{\varphi}$. Here, $\overline{G}$ denotes the complement graph of G. Roughly speaking, a fragment/extension L of first-order logic is self-complementary if expressions of the form Exy can be replaced by $\neg Exy \wedge (x \neq y)$ in every formula while remaining in L. This lax requirement is satisfied by many logics including first-order logic, counting logic, second-order logic, fixed-point logics, and bounded variable, quantifier depth, or quantifier prefix fragments of these. All these examples are subject to the following result:

▶ **Theorem 1.** *Let $(\mathsf{L}, \models)$ be a self-complementary logic on graphs for which there exists a graph class $\mathcal{F}$ such that two graphs G and H are homomorphism indistinguishable over $\mathcal{F}$ if and only if they are L-equivalent. Then there exists a minor-closed graph class $\mathcal{F}'$ whose homomorphism indistinguishability relation coincides with L-equivalence.*

Theorem 1 can be used to rule out that a given logic has a homomorphism indistinguishability characterisation (Corollary 17). Furthermore, it allows to use the deep results of graph minor theory to study the expressive power of logics on graphs (Theorem 22).

Theorem 1 is product of a more fundamental study of the properties of homomorphism indistinguishability relations. In several instances, it is shown that closure properties of a graph class $\mathcal{F}$ correspond to preservation properties of its homomorphism indistinguishability relation $\equiv_{\mathcal{F}}$. These efforts yield answers to several open questions from [32]. A prototypical result is Theorem 2, from which Theorem 1 follows. For further results in the same vein concerning other closure properties, e.g. under taking subgraphs, see Table 1.

▶ **Theorem 2.** *Let $\mathcal{F}$ be a homomorphism distinguishing closed graph class. Then $\mathcal{F}$ is minor-closed if and only if $\equiv_{\mathcal{F}}$ is preserved under taking complements, i.e. for all simple graphs G and H it holds that $G \equiv_{\mathcal{F}} H$ if and only if $\overline{G} \equiv_{\mathcal{F}} \overline{H}$.*

Here, the graph class $\mathcal{F}$ is *homomorphism distinguishing closed* [32] if for every $K \notin \mathcal{F}$ there exist graphs G and H which are homomorphism indistinguishable over $\mathcal{F}$ but differ in the number of homomorphisms from K. In other words, adding even a single graph to $\mathcal{F}$ would change its homomorphism indistinguishability relation.

[1] For all $\varphi \in \mathsf{L}$ and graphs G and H such that $G \cong H$, it holds that $G \models \varphi$ iff $H \models \varphi$.

Proving that a graph class is homomorphism distinguishing closed is a pathway to separating equivalence relations comparing graphs [33]. However, establishing this property is a notoriously hard task. Thus, a general result establishing the homomorphism distinguishing closedness of a wide range of graph classes would be desirable. In [32], Roberson conjectured that *every graph class closed under taking minors and disjoint unions is homomorphism distinguishing closed*. At present, this conjecture has only been verified for few graph classes [32, 28].

Our final result confirms Roberson's conjecture for all graph classes which are in a certain sense finite. The expressive power of homomorphism counts from finitely many graphs is of particular importance in practice. Applications include the design of graph kernels [21], motif counting [2, 26], or machine learning on graphs [6, 30, 20]. A theoretical interest stems for example from database theory where homomorphism counts correspond to results of queries under bag-semantics [8, 22], see also [9].

Since every homomorphism distinguishing closed graph class is closed under taking disjoint unions, infinite graph classes arise inevitably when studying homomorphism indistinguishability over finite graph classes. We introduce the notions of *essentially finite* and *essentially profinite* graph classes (Definition 23) in order to capture the nevertheless limited behaviour of graph classes arising from the finite. Examples for essentially profinite graph classes include the class of all minors of a fixed graph and the class of cluster graphs, i.e. disjoint unions of arbitrarily large cliques. In Theorem 24, the essentially profinite graph classes which are homomorphism distinguishing closed are fully classified. Thereby, the realm of available examples of homomorphism distinguishing closed graph classes is drastically enlarged. This classification has the following readily-stated corollary:

▶ **Theorem 3.** *Every essentially profinite union-closed graph class $\mathcal{F}$ which is closed under taking summands*[2] *is homomorphism distinguishing closed. In particular, Roberson's conjecture holds for all essentially profinite graph classes.*

2 Preliminaries

All graphs in this article are finite, undirected, and without multiple edges. A *simple graph* is a graph without loops. A *homomorphism* from a graph F to a graph G is a map $h\colon V(F) \to V(G)$ such that $h(u)h(v) \in E(G)$ whenever $uv \in E(F)$ and vertices carrying loops are mapped to vertices carrying loops. Write $\hom(F, G)$ for the number of homomorphisms from F to G. For a class of graphs $\mathcal{F}$ and graphs G and H, write $G \equiv_{\mathcal{F}} H$ if $\hom(F, G) = \hom(F, H)$ for all $F \in \mathcal{F}$, i.e. G and H are *homomorphism indistinguishable over* $\mathcal{F}$. With the exception of Section 3.2, the graphs in $\mathcal{F}$, G and H will be simple. Following [32], the *homomorphism distinguishing closure* of $\mathcal{F}$ is

$$\operatorname{cl}(\mathcal{F}) \coloneqq \{K \text{ simple graph} \mid \forall \text{ simple graphs } G, H. \quad G \equiv_{\mathcal{F}} H \Rightarrow \hom(K, G) = \hom(K, H)\}.$$

Intuitively, $\operatorname{cl}(\mathcal{F})$ is the 'largest' graph class whose homomorphism indistinguishability relation coincides with the one of $\mathcal{F}$. A graph class $\mathcal{F}$ is *homomorphism distinguishing closed* if $\operatorname{cl}(\mathcal{F}) = \mathcal{F}$. Note that cl is a closure operator in the sense that $\operatorname{cl}(\mathcal{F}) \subseteq \operatorname{cl}(\mathcal{F}')$ if $\mathcal{F} \subseteq \mathcal{F}'$ and $\operatorname{cl}(\operatorname{cl}(\mathcal{F})) = \operatorname{cl}(\mathcal{F})$ for all graph classes $\mathcal{F}$ and $\mathcal{F}'$.

For graphs G and H, write $G + H$ for their *disjoint union* and $G \times H$ for their *categorical product*, i.e. $V(G \times H) \coloneqq V(G) \times V(H)$ and gh and $g'h'$ are adjacent in $G \times H$ iff $gg' \in E(G)$ and $hh' \in E(H)$. The *lexicographic product* $G \cdot H$ is defined as the graph with vertex set

[2] A graph class $\mathcal{F}$ is *closed under taking summands* if for all $F \in \mathcal{F}$ which is the disjoint union of two graphs $F_1 + F_2 = F$ also $F_1, F_2 \in \mathcal{F}$.

$V(G) \times V(H)$ and edges between gh and $g'h'$ iff $g = g'$ and $hh' \in E(H)$ or $gg' \in E(G)$. It is well-known, cf. e.g. [24, (5.28)–(5.30)], that for all graphs F_1, F_2, G_1, G_2, and all connected graphs K,

$$\hom(F_1 + F_2, G) = \hom(F_1, G) \hom(F_2, G), \tag{1}$$
$$\hom(F, G_1 \times G_2) = \hom(F, G_1) \hom(F, G_2), \text{ and} \tag{2}$$
$$\hom(K, G_1 + G_2) = \hom(K, G_1) + \hom(K, G_2). \tag{3}$$

The *complement* of a simple graph F is the simple graph $\overline{F}$ with $V(\overline{F}) = V(F)$ and $E(\overline{F}) = \binom{V(F)}{2} \setminus E(F)$. Observe that $\overline{\overline{F}} = F$ for all simple graphs F. The *full complement* of a graph G is the graph $\widehat{G}$ obtained from G by replacing every edge with a non-edge and every loop with a non-loop, and vice-versa.

The *quotient* $F/\mathcal{P}$ of a simple graph F by a partition $\mathcal{P}$ of $V(F)$ is the simple graph with vertex set $\mathcal{P}$ and edges PQ for $P \neq Q$ iff there exist vertices $p \in P$ and $q \in Q$ such that $pq \in E(F)$. For a set X, write $\Pi(X)$ for the set of all partitions of X. We do not include loops in order to state Theorem 14 succinctly.

A graph F' can be obtained from a simple graph F by *contracting edges* if there is a partition $\mathcal{P} \in \Pi(V(F))$ such that $F[P]$ is connected for all $P \in \mathcal{P}$ and $F' \cong F/\mathcal{P}$.

For a graph F and a set $P \subseteq V(F)$, write $F[P]$ for the *subgraph induced by* P, i.e. the graph with vertex set P and edges uv if $u, v \in P$ and $uv \in E(F)$. A graph F' is a *subgraph* of F, in symbols $F' \subseteq F$ if $V(F') \subseteq V(F)$ and $E(F') \subseteq E(F)$. A *minor* of a simple graph F is a subgraph of a graph which can be obtained from F by contracting edges.

3 Closure Properties Correspond to Preservation Properties

This section is concerned with the interplay of closure properties of a graph class $\mathcal{F}$ and preservation properties of its homomorphism indistinguishability relation $\equiv_{\mathcal{F}}$. The central results of this section are Theorem 2 and the other results listed in Table 1.

The relevance of the results is twofold: On the one hand, they yield that if a graph class $\mathcal{F}$ has a certain closure property then so does $\mathrm{cl}(\mathcal{F})$. In the case of minor-closed graph families, this provides evidence for Roberson's conjecture [32]. On the other hand, they establish that equivalence relations comparing graphs which are preserved under certain operations coincide with the homomorphism indistinguishability relation over a graph class with a certain closure property, if they are homomorphism indistinguishability relations at all. Further consequences are discussed in Sections 3.5 and 4. Essential to all proofs is the following lemma:

▶ **Lemma 4.** *Let $\mathcal{F}$ and $\mathcal{L}$ be classes of simple graphs. Suppose $\mathcal{L}$ is finite and that its elements are pairwise non-isomorphic. Let $\alpha \colon \mathcal{L} \to \mathbb{R} \setminus \{0\}$. If for all simple graphs G and H*

$$G \equiv_{\mathcal{F}} H \implies \sum_{L \in \mathcal{L}} \alpha_L \hom(L, G) = \sum_{L \in \mathcal{L}} \alpha_L \hom(L, H)$$

then $\mathcal{L} \subseteq \mathrm{cl}(\mathcal{F})$.

Proof. The following argument is due to [11, Lemma 3.6]. Let n be an upper bound on the number of vertices of graphs in $\mathcal{L}$ and let $\mathcal{L}'$ denote the class of all graphs on at most n vertices. By classical arguments [23], the matrix $M := (\hom(K, L))_{K, L \in \mathcal{L}'}$ is invertible. Extend α to a function $\alpha' \colon \mathcal{L}' \to \mathbb{R}$ by setting $\alpha'(L) := \alpha(L)$ for all $L \in \mathcal{L}$ and $\alpha'(L') := 0$ for all $L' \in \mathcal{L}' \setminus \mathcal{L}$. If $G \equiv_{\mathcal{F}} H$ then $G \times K \equiv_{\mathcal{F}} H \times K$ for all graphs K. Hence, by Equation (2),

$$\begin{tikzcd}
& \text{edge contractions} \arrow[rrr, dashed] & & & \text{summands} \\
\text{minors} \arrow[ur] \arrow[r] & \text{edge deletion} \arrow[r, dashed] & \text{subgraphs} \arrow[r] & \text{induced subgraphs} \arrow[ur] &
\end{tikzcd}$$

Figure 1 Relationship between closure properties of homomorphism distinguishing closed graph classes. The non-obvious implications (dashed) are proven in Lemmas 8 and 16.

$$\sum_{L\in\mathcal{L}'} \hom(L,K)\alpha_L \hom(L,G) = \sum_{L\in\mathcal{L}'} \hom(L,K)\alpha_L \hom(L,H).$$

Both sides can be read as the product of the matrix M^T with a vector of the form $(\alpha_L \hom(L,-))_{L\in\mathcal{L}'}$. By multiplying from the left with the inverse of M^T, it follows that $\alpha_L \hom(L,G) = \alpha_L \hom(L,H)$ for all $L \in \mathcal{L}'$ which in turn implies that $\hom(L,G) = \hom(L,H)$ for all $L \in \mathcal{L}$. Thus, $\mathcal{L} \subseteq \mathrm{cl}(\mathcal{F})$. ◀

In the setting of Lemma 4, we say that the relation $\equiv_{\mathcal{F}}$ *determines* the linear combination $\sum_{L\in\mathcal{L}} \alpha_L \hom(L,-)$. Note that it is essential for the argument to carry through that the elements of $\mathcal{L}$ are pairwise non-isomorphic and that $\alpha_L \neq 0$ for all L. Efforts will be undertaken to establish this property for certain linear combinations in the subsequent sections.

3.1 Taking Summands and Preservation under Disjoint Unions

In this section, the strategy yielding the results in Table 1 is presented for the rather simple case of Theorem 5. This theorem relates the property of a graph class $\mathcal{F}$ to be closed under taking summands to the property of $\equiv_{\mathcal{F}}$ to be preserved under disjoint unions. This closure property is often assumed in the context of homomorphism indistinguishability [1, 32] and fairly mild. It is the most general property among those studied here, cf. Figure 1. Theorem 5 answers a question from [32, p. 7] affirmatively: Is it true that if $\equiv_{\mathcal{F}}$ is preserved under disjoint unions then $\mathrm{cl}(\mathcal{F})$ is closed under taking summands?

▶ **Theorem 5.** *For a graph class $\mathcal{F}$ and the assertions*
- **(i)** *$\mathcal{F}$ is closed under taking summands, i.e. if $F_1 + F_2 \in \mathcal{F}$ then $F_1, F_2 \in \mathcal{F}$,*
- **(ii)** *$\equiv_{\mathcal{F}}$ is* preserved under disjoint unions*, i.e. for all simple graphs G, G', H, and H', if $G \equiv_{\mathcal{F}} G'$ and $H \equiv_{\mathcal{F}} H'$ then $G + H \equiv_{\mathcal{F}} G' + H'$,*
- **(iii)** *$\mathrm{cl}(\mathcal{F})$ is closed under taking summands.*

the implications i $\Rightarrow$ ii $\Leftrightarrow$ iii hold.

Proof. The central idea is to write, given graphs F, G, and H, the quantity $\hom(F, G+H)$ as expression in $\hom(F', G)$ and $\hom(F', H)$ where the F' range over summands of F. To this end, write $F = C_1 + \cdots + C_r$ as disjoint union of its connected components. Then,

$$\begin{aligned}
\hom(F, G+H) &\overset{(1)}{=} \prod_{i=1}^{r} \hom(C_i, G+H) \overset{(3)}{=} \prod_{i=1}^{r} (\hom(C_i,G) + \hom(C_i,H)) \\
&\overset{(1)}{=} \sum_{I\subseteq[r]} \hom(\sum_{i\in I} C_i, G) \hom(\sum_{i\in[r]\setminus I} C_i, H).
\end{aligned} \tag{4}$$

In particular, if $\mathcal{F}$ is closed under taking summands then $\sum_{i\in I} C_i \in \mathcal{F}$ for all $I \subseteq [r]$. Thus, i implies ii.

Assume ii and let $F \in \mathrm{cl}(\mathcal{F})$. Write as above $F = C_1 + \dots + C_r$ as disjoint union of its connected components. By the assumption that $\equiv_\mathcal{F}$ is preserved under disjoint unions, for all graphs G and G', if $G \equiv_\mathcal{F} G'$ then $G + F \equiv_\mathcal{F} G' + F$ and hence $\hom(F, G + F) = \hom(F, G' + F)$. By Equation (4) with $H = F$, the relation $\equiv_\mathcal{F}$ determines the linear combination $\sum_{I \subseteq [r]} \hom(\sum_{i \in I} C_i, -) \hom(\sum_{i \in [r] \setminus I} C_i, F)$. Note that it might be the case that $\sum_{i \in I} C_i \cong \sum_{j \in J} C_j$ for some $I \neq J$. Grouping such summands together and adding their coefficients yields a linear combination satisfying the assumptions of Lemma 4 since $\hom(C_i, F) > 0$ for all $i \in [r]$. Hence, $\sum_{i \in I} C_i \in \mathrm{cl}(\mathcal{F})$ for all $I \subseteq [r]$ and iii follows.

The implication iii $\Rightarrow$ ii follows from i $\Rightarrow$ ii for $\mathrm{cl}(\mathcal{F})$ since $\equiv_\mathcal{F}$ and $\equiv_{\mathrm{cl}(\mathcal{F})}$ coincide. ◀

The proofs of the other results in Table 1 are conceptually similar to the just completed proof. The general idea can be briefly described as follows:

1. Derive a linear expression similar to Equation (4) for the number of homomorphisms from F into the graph constructed using the assumed preservation property of $\equiv_\mathcal{F}$, e.g. the graph $G + H$ in the case of Theorem 5. These linear combinations typically involve sums over subsets U of vertices or edges of F, each contributing a summand of the form $\alpha_U \hom(F_U, -)$ where α_U is some coefficient and F_U is a graph constructed from F using U. Hence, if $\mathcal{F}$ is closed under the construction transforming F to F_U then $\equiv_\mathcal{F}$ has the desired preservation property.
2. In general, it can be that F_U and $F_{U'}$ are isomorphic even though $U \neq U'$, e.g. in Equation (4) if F contains two isomorphic connected components. In order to apply Lemma 4, one must group the summands $\alpha_U \hom(F_U, -)$ by the isomorphism type F' of the F_U. The coefficient of $\hom(F', -)$ in the new linear combination ranging over pairwise non-isomorphic graphs is the sum of α_U over all U such that $F_U \cong F'$. Once it is established that this coefficient is non-zero, it follows that if $\equiv_\mathcal{F}$ has the preservation property then $\mathrm{cl}(\mathcal{F})$ has the desired closure property.

3.2 Taking Subgraphs and Preservation under Full Complements

The strategy which yielded Theorem 5 can be extended to obtain the following Theorem 6 relating the property of a graph class $\mathcal{F}$ to be closed under taking subgraphs to the property of $\equiv_\mathcal{F}$ to be preserved under taking full complements.

Since our definition of the homomorphism distinguishing closure involves only simple graph in order to be aligned with [32], Theorem 6 deviates slightly from the other results in Table 1. This is because the relations $\equiv_\mathcal{F}$ and $\equiv_{\mathrm{cl}(\mathcal{F})}$ a priori coincide only on simple graphs and not necessarily on all graphs, a crucial point raised by a reviewer.

▶ **Theorem 6.** *For a graph class $\mathcal{F}$ and the assertions*

(i) *$\mathcal{F}$ is closed under deleting edges,*
(ii) *$\equiv_\mathcal{F}$ is* preserved under taking full complements*, i.e. for all simple graphs G and H it holds that $G \equiv_\mathcal{F} H$ if and only if $\widehat{G} \equiv_\mathcal{F} \widehat{H}$,*
(iii) $\mathrm{cl}(\mathcal{F})$ *is closed under deleting edges,*
(iv) $\mathrm{cl}(\mathcal{F})$ *is closed under taking subgraphs, i.e. it is closed under deleting edges and vertices,*
(v) *$\equiv_{\mathrm{cl}(\mathcal{F})}$ is preserved under taking full complements,*

the implications i $\Rightarrow$ ii $\Rightarrow$ iii $\Leftrightarrow$ iv $\Leftrightarrow$ v hold.

The linear expression required by Lemma 4 is provided by the following Lemma 7 based on the Inclusion–Exclusion principle. That iii implies iv follows from the Lemma 8. The proofs are deferred to the full version [35].

▶ **Lemma 7** ([24, Equation (5.23)])**.** *For every simple graph F and graph G,*

$$\hom(F, \widehat{G}) = \sum_{F' \subseteq F \text{ s.t. } V(F') = V(F)} (-1)^{|E(F')|} \hom(F', G).$$

▶ **Lemma 8.** *If a homomorphism distinguishing closed graph class $\mathcal{F}$ is closed under deleting edges then it is closed under taking subgraphs.*

3.3 Taking Minors and Preservation under Complements

The insights gained in the previous sections are now orchestrated to prove Theorem 9, which implies Theorem 2. This answers a question of Roberson [32, Question 8] affirmatively: Is it true that if $\mathcal{F}$ is such that $\equiv_{\mathcal{F}}$ is preserved under taking complements then there exist a minor-closed $\mathcal{F}'$ such that $\equiv_{\mathcal{F}}$ and $\equiv_{\mathcal{F}'}$ coincide.

Theorem 9 is among the first results substantiating Roberson's conjecture not only for example classes but in full generality. In particular, as noted in [32, p. 2], there was little reason to believe that minor-closed graph families should play a distinct role in the theory of homomorphism indistinguishability. Theorem 9 indicates that this might be the case. Indeed, while Roberson's conjecture asserts that $\mathrm{cl}(\mathcal{F})$ coincides with $\mathcal{F}$ for a minor-closed and union-closed graph class $\mathcal{F}$, Theorem 9 yields unconditionally that $\mathrm{cl}(\mathcal{F})$ is a minor-closed graph class itself.

▶ **Theorem 9.** *For a graph class $\mathcal{F}$ and the assertions*

(i) *$\mathcal{F}$ is closed under edge contraction and deletion,*

(ii) *$\equiv_{\mathcal{F}}$ is preserved under taking complements, i.e. for all simple graphs G and H it holds that $G \equiv_{\mathcal{F}} H$ if and only if $\overline{G} \equiv_{\mathcal{F}} \overline{H}$,*

(iii) *$\mathrm{cl}(\mathcal{F})$ is minor-closed,*

the implications $i \Rightarrow ii \Leftrightarrow iii$ hold.

Again, the strategy is to write $\hom(F, \overline{G})$ as a linear combination of $\hom(F', G)$ for minors F' of F. For a simple graph G, write G° for the graph obtained from G by adding a loop to every vertex. In light of Lemma 7, which concerns $\hom(F, \widehat{G})$, noting that $\widehat{G^\circ} \cong \overline{G}$ for every simple graph G, it suffices to write $\hom(F, G^\circ)$ as a linear combination of $\hom(F', G)$ for minors F' of F. To that end, we consider a particular type of quotient graphs.

For a simple graph F and a set of edges $L \subseteq E(F)$, define the *contraction relation* $\sim_L$ on $V(F)$ by declaring $v \sim_L w$ if v and w lie in the same connected component of the subgraph of F with vertex set $V(F)$ and edge set L. Write $[v]_L$ for the classes of $v \in V(F)$ under the equivalence relation $\sim_L$.

The *contraction quotient* $F \oslash L$ is the graph whose vertex set is the set of equivalence classes under $\sim_L$ and with an edge between $[v]_L$ and $[w]_L$ if and only if there is an edge $xy \in E(F) \setminus L$ such that $x \sim_L v$ and $y \sim_L w$. In general, $F \oslash L$ may contain loops, cf. Example 11. However, if it is simple then it is equal to $F/\mathcal{P}$ where $\mathcal{P}$ is the partition of $V(F)$ into equivalence classes under $\sim_L$, i.e. $\mathcal{P} \coloneqq \{[v]_L \mid v \in V(F)\}$. In this case, $F \oslash L$ is a graph obtained from F by edge contractions.

With this notation, the quantity $\hom(F, G^\circ)$ can be succinctly written as linear combination. Using Proposition 10 and Lemma 7, Theorem 9 can be proven by the strategy described in Section 3.1. The proofs are deferred to [35].

▶ **Proposition 10.** *Let F and G be simple graphs. Then*

$$\hom(F, G^\circ) = \sum_{L \subseteq E(F)} \hom(F \oslash L, G).$$

▶ **Example 11.** Let K_3 denote the clique with vertex set $\{1, 2, 3\}$. Then $K_3 \oslash \emptyset \cong K_3$, $K_3 \oslash \{12\} \cong K_2$, $K_3 \oslash \{12, 23\} \cong K_1^\circ$, and $K_3 \oslash \{12, 23, 13\} \cong K_1$. For every simple graph G, $\hom(K_3, G^\circ) = \hom(K_3, G) + 3\hom(K_2, G) + \hom(K_1, G)$ since $\hom(K_1^\circ, G) = 0$.

3.4 Taking Induced Subgraphs, Contracting Edges, and Lexicographic Products

In this section, it is shown that a homomorphism distinguishing closed graph class is closed under taking induced subgraphs (contracting edges) if and only if its homomorphism indistinguishability relation is preserved under lexicographic products with a fixed graph from the left (from the right).

Examples for equivalence relations preserved under lexicographic products related to chromatic graph parameters are listed in Corollary 18. Further examples are of model-theoretic nature and stem from winning strategies of the Duplicator player in bijective pebble games [35].

▶ **Theorem 12.** *For a graph class $\mathcal{F}$ and the assertions*

(i) *$\mathcal{F}$ is closed under taking induced subgraphs,*

(ii) *$\equiv_{\mathcal{F}}$ is such that for all simple graphs G, H, H', if $H \equiv_{\mathcal{F}} H'$ then $G \cdot H \equiv_{\mathcal{F}} G \cdot H'$,*

(iii) *$\mathrm{cl}(\mathcal{F})$ is closed under taking induced subgraphs.*

the implications $i \Rightarrow ii \Leftrightarrow iii$ hold.

An example for a lexicographic product from the right is the *n-blow-up* $G \cdot \overline{K_n}$ of a graph G. It can be seen [24] that every homomorphism indistinguishability relation is preserved under blow-ups. Preservation under arbitrary lexicographic products from the right, however, is a non-trivial property corresponding to the associated graph class being closed under edge contractions:

▶ **Theorem 13.** *For a graph class $\mathcal{F}$ and the assertions*

(i) *$\mathcal{F}$ is closed under edge contractions,*

(ii) *$\equiv_{\mathcal{F}}$ is such that for all simple graphs G, G', H, if $G \equiv_{\mathcal{F}} G'$ then $G \cdot H \equiv_{\mathcal{F}} G' \cdot H$,*

(iii) *$\mathrm{cl}(\mathcal{F})$ is closed under edge contractions.*

the implications $i \Rightarrow ii \Leftrightarrow iii$ hold.

For the proofs, homomorphism counts $\hom(F, G \cdot H)$ are written as linear combinations of homomorphism counts $\hom(F', H)$ where F' ranges over induced subgraphs of F in the case of Theorem 12 and over graphs obtained from F' by contracting edges in the case of Theorem 13. The following succinct formula for counts of homomorphisms into a lexicographic product is derived in the full version [35]. It may be of independent interest.

▶ **Theorem 14.** *Let F, G, and H be simple graphs. Then*

$$\hom(F, G \cdot H) = \sum_{\mathcal{R}} \hom(F/\mathcal{R}, G) \hom(\sum_{R \in \mathcal{R}} F[R], H)$$

where the outer sum ranges over all $\mathcal{R} \in \Pi(V(F))$ such that $F[R]$ is connected for all $R \in \mathcal{R}$.

Theorem 14 yields Theorems 12 and 13, which in turn imply together the following Corollary 15. The proofs are deferred to the full version [35].

▶ **Corollary 15.** *For a graph class $\mathcal{F}$ and the assertions*

(i) *$\mathcal{F}$ is closed under taking induced subgraphs and edge contractions,*

(ii) *$\equiv_{\mathcal{F}}$ is such that for all simple graphs G, G', H, and H', if $G \equiv_{\mathcal{F}} G'$ and $H \equiv_{\mathcal{F}} H'$ then $G \cdot H \equiv_{\mathcal{F}} G' \cdot H'$,*

(iii) *$\mathrm{cl}(\mathcal{F})$ is closed under taking induced subgraphs and edge contractions.*

the implications $i \Rightarrow ii \Leftrightarrow iii$ hold.

As a final observation, the following Lemma 16 relates the property of being closed under edge contractions to the other closure properties in Table 1.

▶ **Lemma 16.** *If a homomorphism distinguishing closed graph class $\mathcal{F}$ is closed under contracting edges then it is closed under taking summands.*

3.5 Applications

As applications of Theorems 6, 9, 12, and 13, we conclude, in the spirit of [3], that certain equivalence relations on graphs cannot be homomorphism distinguishing relations.

▶ **Corollary 17.** *Let $\mathcal{F}$ be a non-empty graph class such that one of the following holds:*

- *$\equiv_{\mathcal{F}}$ is preserved under complements, cf. Theorem 9,*
- *$\equiv_{\mathcal{F}}$ is preserved under full complements, cf. Theorem 6,*
- *$\equiv_{\mathcal{F}}$ is preserved under left lexicographic products, cf. Theorem 12, or*
- *$\equiv_{\mathcal{F}}$ is preserved under right lexicographic products, cf. Theorem 13.*

Then $G \equiv_{\mathcal{F}} H$ implies that $|V(G)| = |V(H)|$ for all graphs G and H.

Proof. By Theorems 6, 9, 12, and 13, $\mathcal{F}$ can be chosen to be closed under taking minors, subgraphs, induced subgraphs, or contracting edges. In any case, $K_1 \in \mathcal{F}$ as $\mathcal{F}$ is non-empty and hence $|V(G)| = \hom(K_1, G) = \hom(K_1, H) = |V(H)|$. ◀

As concrete examples, consider the following relations.

▶ **Corollary 18.** *There is no graph class $\mathcal{F}$ satisfying any of the following assertions for all graphs G and H:*

(i) *$G \equiv_{\mathcal{F}} H$ iff $a(G) = a(H)$ where a denotes the order of the automorphism group,*
(ii) *$G \equiv_{\mathcal{F}} H$ iff $\alpha(G) = \alpha(H)$ where α denotes the size of the largest independent set,*
(iii) *$G \equiv_{\mathcal{F}} H$ iff $\omega(G) = \omega(H)$ where ω denotes the size of the largest clique,*
(iv) *$G \equiv_{\mathcal{F}} H$ iff $\chi(G) = \chi(H)$ where χ denotes the chromatic number.*

Proof. The relation in Item i is preserved under taking complements. By [17, Theorem 1, Corollary p. 90], the relations in Items ii and iv are preserved under left lexicographic products. For Item iii, the same follows from [17, Theorem 1] observing that $\overline{G} \cdot \overline{H} = \overline{G \cdot H}$ and $\omega(G) = \alpha(\overline{G})$. In each case, it is easy to exhibit a pair of graphs G and H in the same equivalence class with different number of vertices. By Corollary 17, none of the equivalence relations is a homomorphism indistinguishability relation. ◀

4 Equivalences over Self-Complementary Logics

In this section, Theorem 1 is derived from Theorem 9. The theorem applies to self-complementary logics, of which examples are given subsequently. Finally, a result from graph minor theory is used to relate logics on graphs to quantum isomorphism.

▶ **Theorem 1.** *Let $(\mathsf{L}, \models)$ be a self-complementary logic on graphs for which there exists a graph class $\mathcal{F}$ such that two graphs G and H are homomorphism indistinguishable over $\mathcal{F}$ if and only if they are L-equivalent. Then there exists a minor-closed graph class $\mathcal{F}'$ whose homomorphism indistinguishability relation coincides with L-equivalence.*

Proof. It is shown that $\equiv_{\mathcal{F}}$ is preserved under taking complements in the sense of Theorem 9. Suppose $G \equiv_{\mathcal{F}} H$. By assumption, for all $\varphi \in \mathsf{L}$ it holds that $G \models \varphi$ iff $H \models \varphi$ and hence, by self-complementarity,

$$\overline{G} \models \varphi \iff G \models \overline{\varphi} \iff H \models \overline{\varphi} \iff \overline{H} \models \overline{\overline{\varphi}} \iff \overline{H} \models \varphi.$$

Here, the penultimate equivalence holds since $H \models \varphi$ if and only if $H \models \overline{\overline{\varphi}}$ for all φ and H by the definition of self-complementarity observing that $\overline{\overline{H}} \cong H$. Thus, $\overline{G} \equiv_{\mathcal{F}} \overline{H}$. By Theorem 9, $\mathcal{F}' \coloneqq \mathrm{cl}(\mathcal{F})$ is minor-closed. ◀

In particular, by Corollary 17, all L-equivalent graphs G and H must have the same number of vertices unless L is trivial in the sense that all graphs G and H are L-equivalent.

A first example of a self-complementarity logic is first-order logic FO over the signature of graphs $\{E\}$. In order to establish this property, a formula $\overline{\varphi} \in \mathsf{FO}$ has to be constructed for every $\varphi \in \mathsf{FO}$ such that $G \models \varphi$ iff $\overline{G} \models \overline{\varphi}$ for all graphs G. Only subformulae Exy require non-trivial treatment:

▶ **Definition 19.** *For every $\varphi \in \mathsf{FO}$, define $\overline{\varphi} \in \mathsf{FO}$ inductively as follows:*

1. *if $\varphi = Exy$ then $\overline{\varphi} \coloneqq \neg Exy \wedge (x \neq y)$,*
2. *if $\varphi = \bot$ or $\varphi = \top$ then $\overline{\varphi} \coloneqq \varphi$, if $\varphi = (x = y)$ then $\overline{\varphi} \coloneqq \varphi$, if $\varphi = \neg\psi$ then $\overline{\varphi} \coloneqq \neg\overline{\psi}$, if $\varphi = \psi \wedge \chi$ then $\overline{\varphi} \coloneqq \overline{\psi} \wedge \overline{\chi}$, if $\varphi = \psi \vee \chi$ then $\overline{\varphi} \coloneqq \overline{\psi} \vee \overline{\chi}$, if $\varphi = \exists x.\ \psi$ then $\overline{\varphi} \coloneqq \exists x.\ \overline{\psi}$, and if $\varphi = \forall x.\ \psi$ then $\overline{\varphi} \coloneqq \forall x.\ \overline{\psi}$.*

▶ **Lemma 20.** *Let $\varphi \in \mathsf{FO}$ be a formula with $k \geq 0$ free variables. Then for all simple graphs G with $\boldsymbol{v} \in V(G)^k$ it holds that*

$$G, \boldsymbol{v} \models \varphi \iff \overline{G}, \boldsymbol{v} \models \overline{\varphi}.$$

In particular, FO is self-complementary.

Proof. The proof is by induction on the structure of φ. If φ is Exy, observe that $v_1v_2 \in E(G)$ if and only if $v_1v_2 \notin E(\overline{G})$ and $v_1 \neq v_2$. In all other cases, the claim is purely syntactical. ◀

Lemma 20 gives a purely syntactical criterion for a fragment $\mathsf{L} \subseteq \mathsf{FO}$ to be self-complementary. Indeed, if $\overline{\varphi} \in \mathsf{L}$ as defined in Definition 19 for all $\varphi \in \mathsf{L}$ then L is self-complementary. Note that the operation in Definition 19 increases neither the number of variables nor affects the quantifiers in the formula. Thus, Lemma 20 automatically extends to fragments of FO defined by restricting the number of variables, order or number of quantifiers. For extensions of FO, Definition 19 can be easily extended, cf. [35]. This yields a rich realm of self-complementary logics, of which the following Example 21 lists only a selection.

▶ **Example 21.** The following logics on graphs are self-complementary. For every $k, d \geq 0$,

- the k-variable and quantifier-depth-d fragments FO^k and FO_d of FO,
- first-order logic with counting quantifiers C and its k-variable and quantifier-depth-d fragments C^k and C_d,
- inflationary fixed-point logic IFP, cf. [18],
- second-order logic SO and its fragments monadic second-order logic MSO_1, existential second-order logic ESO, cf. [10, 16].

Corollary 17 readily gives an alternative proof of [3, Propositions 1 and 2], which assert that neither FO^k-equivalence nor FO_d-equivalence are characterised by homomorphism indistinguishability relations. The logic fragments C^k and C_d are however characterised by homomorphism indistinguishability relations [14, 19].

The final result of this section demonstrates how graph minor theory can yield insights into the expressive power of logics via Theorem 1. Subject to it are self-complementary logics which have a homomorphism indistinguishability characterisation and are stronger than C^k for every k, e.g. they are capable of distinguishing CFI-graphs [7]. It is shown that equivalence w.r.t. any such logic is a sufficient condition for quantum isomorphism, an undecidable equivalence comparing graphs [4].

▶ **Theorem 22.** *Let* $(\mathsf{L}, \models)$ *be a self-complementary logic on graphs for which there exists a graph class* $\mathcal{F}$ *such that two graphs* G *and* H *are homomorphism indistinguishable over* $\mathcal{F}$ *if and only if they are* L*-equivalent. Suppose that for all* $k \in \mathbb{N}$ *there exist graphs* G *and* H *such that* $G \equiv_{\mathsf{C}^k} H$ *and* $G \not\equiv_{\mathsf{L}} H$*. Then all* L*-equivalent graphs are quantum isomorphic.*

Proof. Contrapositively, it is shown that if there exist non-quantum-isomorphic L-equivalent graphs then there exists a $k \in \mathbb{N}$ such that $G \equiv_{\mathsf{C}^k} H \implies G \equiv_{\mathsf{L}} H$ for all G and H. By [25, 14], this statement can be rephrased in the language of homomorphism indistinguishability as $\mathcal{P} \not\subseteq \mathrm{cl}(\mathcal{F}) \implies \exists k \in \mathbb{N}.\ \mathcal{F} \subseteq \mathrm{cl}(\mathcal{TW}_k)$ where $\mathcal{P}$ denotes the class of all planar graphs and $\mathcal{TW}_k$ the class of all graphs of treewidth at most k. By Theorem 9, $\mathrm{cl}(\mathcal{F})$ is a minor-closed graph class. By [34, (2.1)], cf. [29, Theorem 3.8], if $\mathrm{cl}(\mathcal{F})$ does not contain all planar graphs then it is of bounded treewidth. Hence, there exists a $k \in \mathbb{N}$ such that $\mathcal{F} \subseteq \mathrm{cl}(\mathcal{F}) \subseteq \mathcal{TW}_k \subseteq \mathrm{cl}(\mathcal{TW}_k)$. ◀

5 Classification of Homomorphism Distinguishing Closed Essentially Profinite Graph Classes

The central result of this section is a classification of the homomorphism distinguishing closed graph classes which are in a sense finite. Since every homomorphism distinguishing closed graph class is closed under disjoint unions, infinite graph classes arise naturally when studying the semantic properties of the homomorphism indistinguishability relations of finite graph classes. Nevertheless, the infinite graph classes arising in this way are *essentially finite*, i.e. they exhibit only finitely many distinct connected components. One may generalise this definition slightly by observing that all graphs F admitting a homomorphism into some fixed graph G have chromatic number bounded by the chromatic number of G. Thus, in order to make a graph class $\mathcal{F}$ behave much like an essentially finite class, it suffices to impose a finiteness condition, for every graph K, on the subfamily of all K-colourable graphs in $\mathcal{F}$.

Formally, for a graph F, write $\Gamma(F)$ for the set of connected components of F. For a graph class $\mathcal{F}$, define $\Gamma(\mathcal{F})$ as the union of the $\Gamma(F)$ where $F \in \mathcal{F}$. For a graph class $\mathcal{F}$ and a graph K, define $\mathcal{F}_K \coloneqq \{F \in \mathcal{F} \mid \hom(F, K) > 0\}$, the set of K-colourable graphs in $\mathcal{F}$.

▶ **Definition 23.** *A graph class* $\mathcal{F}$ *is* essentially finite *if* $\Gamma(\mathcal{F})$ *is finite. It is* essentially profinite *if* $\mathcal{F}_K$ *is essentially finite for all graphs* K*.*

Clearly, every finite graph class is essentially finite and hence essentially profinite. Other examples for essentially profinite classes are the class of all cliques. They represent a special case of the following construction from [32, Theorem 6.16]: For every $S \subseteq \mathbb{N}$, the family

$$\mathcal{K}^S \coloneqq \{K_{n_1} + \dots + K_{n_r} \mid r \in \mathbb{N}, \{n_1, \dots, n_r\} \subseteq S\} \tag{5}$$

is essentially profinite. In particular, there are uncountably many such families of graphs. Note that one may replace the sequence of cliques $(K_n)_{n\in\mathbb{N}}$ in Equation (5) by any other sequence of connected graphs $(F_n)_{n\in\mathbb{N}}$ such that the sequence of chromatic numbers $(\chi(F_n))_{n\in\mathbb{N}}$ takes every value only finitely often.

Every graph F of an essentially finite family $\mathcal{F}$ can be represented uniquely as vector $\vec{F} \in \mathbb{R}^{\Gamma(\mathcal{F})}$ whose C-th entry for $C \in \Gamma(\mathcal{F})$ is the number of times the graph C appears as a connected component in F. The classification of the homomorphism distinguishing closed essentially profinite graph classes can now be stated as follows. The proof, deferred to the full version [35], is based on a generalisation of a result by Kwiecień, Marcinkowski, and Ostropolski-Nalewaja [22].

▶ **Theorem 24.** *For an essentially profinite graph class $\mathcal{F}$, the following are equivalent:*

(i) *$\mathcal{F}$ is homomorphism distinguishing closed,*

(ii) *For every graph K, if $\vec{K} \in \operatorname{span}\{\vec{F} \in \mathbb{R}^{\Gamma(\mathcal{F}_K \cup \{K\})} \mid F \in \mathcal{F}_K\}$ then $K \in \mathcal{F}$,*

(iii) *$\mathcal{F}_K$ is homomorphism distinguishing closed for every graph K.*

Theorem 24 directly implies Theorem 3. Indeed, if $\mathcal{F}$ is union-closed and closed under summands then $\Gamma(\mathcal{F}) \subseteq \mathcal{F}$ and every graph K such that $\Gamma(K) \subseteq \Gamma(\mathcal{F})$ is itself in $\mathcal{F}$. In particular, Theorem 24 implies that all essentially profinite union-closed minor-closed graph classes are homomorphism distinguishing closed. For example, for every graph G, the union-closure of the class of minors of G is homomorphism distinguishing closed.

To demonstrate the inner workings of condition ii in Theorem 24, we consider the following examples. The first example shows that not even the weakest closure property from Figure 1 is shared by all homomorphism distinguishing closed families. The second example answers a question from [32, p. 29] negatively: Is the disjoint union closure of the union of homomorphism distinguishing closed families homomorphism distinguishing closed?

▶ **Example 25.** Let F_1, F_2 be connected non-isomorphic graphs such that $\hom(F_1, F_2) > 0$.

1. The class $\mathcal{F}_1 \coloneqq \{n(F_1 + F_2) \mid n \geq 1\}$ is homomorphism distinguishing closed and not closed under taking summands.
2. For the homomorphism distinguishing closed $\mathcal{F}_2 \coloneqq \{nF_1 \mid n \geq 1\}$, the disjoint union closure of $\mathcal{F}_1 \cup \mathcal{F}_2$ is not homomorphism distinguishing closed.

Some further enjoyable properties of essentially (pro)finite graph classes merit being commented on. Statements and proofs are deferred to the full version [35]. Firstly, the homomorphism indistinguishability relation of no essentially profinite graph class is as fine as the isomorphism relation $\cong$. This is because the homomorphism distinguishing closure of an essentially profinite graph class is essentially profinite. Secondly, the complexity-theoretic landscape of the problem $\textsc{HomInd}(\mathcal{F})$ of deciding whether two graphs G and H are homomorphism indistinguishable over an essentially profinite class $\mathcal{F}$ is rather diverse. For essentially finite $\mathcal{F}$, $\textsc{HomInd}(\mathcal{F})$ is in polynomial time. For essentially profinite $\mathcal{F}$, the problem can be arbitrarily hard.

6 Conclusion

The main technical contribution of this work is a characterisation of closure properties of graph classes $\mathcal{F}$ in terms of preservation properties of their homomorphism indistinguishability relations $\equiv_{\mathcal{F}}$, cf. Table 1. In consequence, a surprising connection between logical equivalences and homomorphism indistinguishability over minor-closed graph classes is established. In this way, results from graph minor theory are made available to the study of the expressive power of logics on graphs. Finally, a full classification of the homomorphism distinguishing closed graph classes which are essentially profinite is given. Various open questions of [32] are answered by results clarifying the properties of homomorphism indistinguishability relations and of the homomorphism distinguishing closure.

It is tempting to view the results in Table 1 as instances of a potentially richer connection between graph-theoretic properties of $\mathcal{F}$ and *polymorphisms* of $\equiv_{\mathcal{F}}$, i.e. isomorphism-invariant maps $\mathfrak{f}$ sending tuples of graphs to graphs such that $\mathfrak{f}(G_1, \dots, G_k) \equiv_{\mathcal{F}} \mathfrak{f}(H_1, \dots, H_k)$ whenever $G_i \equiv_{\mathcal{F}} H_i$ for all $i \in [k]$. Recalling the algebraic approach to CSPs, cf. [5], one may ask what structural insights into $\mathcal{F}$ can be gained by considering polymorphisms of $\equiv_{\mathcal{F}}$. More concretely, can bounded treewidth or closure under topological minors be characterised in terms of some polymorphism?

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