Equality on all #CSP Instances Yields Constraint Function Isomorphism via Interpolation and Intertwiners

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Abstract

A fundamental result in the study of graph homomorphisms is Lovász's theorem that two graphs are isomorphic if and only if they admit the same number of homomorphisms from every graph. Cai and Govorov capped a line of work extending Lovász's result to more general types of graphs by showing that it holds for graphs with vertex and edge weights from an arbitrary field of characteristic zero. Counting graph homomorphisms is a counting constraint satisfaction problem (#CSP) parameterized by a single constraint function of arity two. In this work, we extend Lovász's theorem to general #CSP by showing that any two sets $\mathcal{F}$ and $\mathcal{G}$ of constraint functions are isomorphic if and only if they are #CSP-indistinguishable – that is, the partition function value of any #CSP instance is unchanged when we replace the functions in $\mathcal{F}$ with those in $\mathcal{G}$. We give two very different proofs of this result. First, we give a proof for complex-valued constraint functions using the intertwiners of the automorphism group of a constraint function set, a concept from the representation theory of compact groups, in the style of Mančinska and Roberson's proof of the equivalence between quantum isomorphism and homomorphism indistinguishability over planar graphs. Second, we demonstrate the power of the simple Vandermonde interpolation technique of Cai and Govorov by extending it to general #CSP, giving a constructive proof for constraint functions with entries from any field of characteristic zero.

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1 Introduction

Graph homomorphisms A homomorphism from (unweighted, undirected) graph K to graph X is a map from the vertex set of K to the vertex set of X which preserves adjacency: every edge of K is mapped to an edge of X. Since Lovász's introduction of graph homomorphisms [25], counting the number $\hom(K, X)$ of homomorphisms from K to X

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has emerged as a well-studied problem in combinatorics and theoretical computer science. One can express $\hom(K, X)$ as the evaluation of a *partition function*, parameterized by X, on K:

$$\hom(K, X) = \sum_{\phi: V(K) \to V(X)} \prod_{(u,v) \in E(K)} (A_X)_{\phi(u),\phi(v)}, \tag{1}$$

where A_X is the adjacency matrix of X. The partition function perspective leads to extensions of graph homomorphism to weighted and directed graphs, as well as a natural view of graph homomorphism as a special case of counting constraint satisfaction problems, or #CSP.

Counting complexity and #CSP Let $\mathbb{F}$ be a field of characteristic zero. A #CSP($\mathcal{F}$) problem is parameterized by a set $\mathcal{F}$ of $\mathbb{F}$-valued *constraint functions* on one or more inputs from a finite *domain* $V(\mathcal{F})$. That is, $F \in \mathcal{F}$ is a function $V(\mathcal{F})^n \to \mathbb{F}$, where n is the *arity* of F. The input to the problem is a #CSP *instance*, consisting of a multiset C of constraints and set V of variables, with each constraint applying a constraint function in $\mathcal{F}$ to a subset of V. The output is the value of the partition function, the sum over all assignments $V \to V(\mathcal{F})$ of the product of the constraint evaluations (see Section 2 for formal definitions). Letting $\mathcal{F} := \{A_X\}$, $V(\mathcal{F}) := V(X)$, $V := V(K)$, and $C := E(K)$, with each edge-constraint applying A_X to its two endpoints, one can see from the partition function formulation of graph homomorphism (1) that counting homomorphisms from K to X is the special case of #CSP($\mathcal{F}$) on instance K where $\mathcal{F}$ contains a single binary (arity-2) constraint function A_X.

Counting graph homomorphisms is a central problem in counting complexity, both in its own right and as a special case of #CSP. Both settings have seen significant dichotomy theorems classifying the partition function as either tractable or #P-hard to compute, depending on X or $\mathcal{F}$, respectively. Graph homomorphism dichotomies have been established for unweighted graphs [17], nonnegative-real-weighted graphs [5, 9], real-weighted graphs [20], and complex-weighted graphs [10]. For #CSP, dichomies have been established for sets of 0-1 valued constraint functions [6, 18], nonnegative-real-valued constraint functions [11], and complex-valued constraint functions [8].

Extending the notion of graph isomorphism, say two constraint functions F and G of the same arity n are isomorphic if there is a bijection $\sigma : V(F) \to V(G)$ such that $F(x_1, \ldots, x_n) = G(\sigma(x_1), \ldots, \sigma(x_n))$ for all $x_1, \ldots, x_n \in V(F)$. Two sets $\mathcal{F}$ and $\mathcal{G}$ of constraint functions are isomorphic ($\mathcal{F} \cong \mathcal{G}$) if there is a bijection $\xi : \mathcal{F} \to \mathcal{G}$ such that there is a common isomorphism between each $F \in \mathcal{F}$ and the corresponding $G = \xi(F) \in \mathcal{G}$. Some similar concepts exist: Böhler et al. [2, 3] study "constraint isomorphism" between Boolean #CSP *instances* (rather than constraint functions), involving permuting variables (rather than domain elements). One can also view an n-ary constraint function F as a tensor in $(\mathbb{F}^{V(F)})^{\otimes n}$; from this perspective the notion of tensor isomorphism [22] is a relaxation of constraint function isomorphism from a bijection $V(F) \to V(G)$ to an invertible linear transformations $\mathbb{F}^{V(F)} \to \mathbb{F}^{V(G)}$.

Homomorphism indistinguishablity. The notion of graph homomorphism naturally extends to directed edge-weighted graphs X by using the weighted adjacency matrix A_X

in (1). Lovász, Freedman, and Schrijver [19, 26, 27] studied the problem of counting homomorphisms to graphs with a real weight assigned to each edge and a nonnegative real weight assigned to each vertex. Lovász [26] extended to these weighted graphs his result, proved forty years prior [25], that two graphs X and Y are isomorphic if and only if they are *homomorphism-indistinguishable*, meaning $\hom(K, X) = \hom(K, Y)$ for every graph K. Throughout this paper, we will refer to such generalizations of Lovász's original theorem as "homomorphism indistinguishability theorems". Lovász's proof for real-weighted graphs [26] used *graph algebras* of formal $\mathbb{C}$-linear combinations of *k-labeled graphs* (which we generalize to k-labeled #CSP instances in Definition 4). Still using k-labeled graphs, but applying invariant theory and algebraic geometry, Schrijver [31] proved a homomorphism indistinguishability theorem for graphs with complex edge weights but without vertex weights. Using similar techniques, Regts [29] proved a homomorphism indistinguishability theorem for graphs with arbitrary vertex and edge weights, provided that no nonempty subset of vertex weights sums to zero. Finally, Cai and Govorov [12] extended the previous results to graphs with any vertex and edge weights from a field $\mathbb{F}$ of characteristic 0, and provide a counterexample to the existence of such a theorem for graphs with weights from any field of nonzero characteristic. Cai and Govorov overcame the algebraic approaches' technical difficulties of vertex weights summing to 0 by applying a simple, direct *Vandermonde interpolation* technique, dependent only on the fact that a Vandermonde matrix with distinct roots is nonsingular. It is remarkable that such a simple tool unifies all previous homomorphism indistinguishability theorems; in Section 4 we further demonstrate its power by using it to extend Cai and Govorov's results to #CSP.

Another line of work uses invariance of homomorphism counts *from* restricted classes of graphs – rather than homomorphisms *to* expanded classes as above – to characterize relaxations of graph isomorphism. Dvořák [16] (see also [27]) showed that homomorphism count from 2-degenerate graphs suffices to determine a graph up to isomorphism, and that homomorphism count from graphs of treewidth at most k determines graphs up to their k-degree refinements, but not up to isomorphism. Dell, Grohe, and Rattan [15] showed that two graphs admit the same number of homomorphisms from all graphs of treewidth at most k if and only if they are indistinguishable by the k-dimensional Weisfeiler-Leman algorithm. Grohe, Rattan, and Seppelt [24] characterize homomorphism indistinguishability over graphs of bounded pathwidth and treedepth in terms of relaxations of linear systems defining isomorphism (see also [23, 30]).

Mančinska and Roberson [28] showed that two graphs are *quantum isomorphic*, an abstract relaxation of isomorphism, if and only if they are homomorphism-indistinguishable over all planar graphs. Their proof uses *quantum permutation groups*, in particular the quantum automorphism group of a graph, analogous to the classical automorphism group. A key component of the proof is Woronowicz's *Tannaka-Krein duality* [32], which implies that every quantum permutation group, a highly abstract object, is uniquely determined by its much more concrete *intertwiner space*. A 'classical' version of Tannaka-Krein duality (Theorem 18) similarly applies to the intertwiner space of the classical automorphism group of a graph, or, more generally, of a set of constraint functions. Using this, we in Section 3 give a classical intertwiner-based proof of our main result Theorem 8 – the same result as proved via Vandermonde interpolation in Section 4, but restricted to sets of constraint functions over $\mathbb{C}$, rather than general fields. Our proof, carried out in the Holant framework from counting complexity (see Section 3.1 below for the definition of Holant) parallels an extension by Cai and Young [13] of Mančinska and Roberson's original 'quantum' result from graph homomorphism to #CSP. The present work is, to our knowledge, the first application of such representation-theoretic techniques to prove a 'classical' indistinguishability theorem. Then Young [34], building on an earlier version of the present work [33], gave an intertwiner-based proof of another such theorem, stating that real-valued $\mathcal{F}$ and $\mathcal{G}$ are equivalent up to orthogonal transformation (a relaxation of isomorphism) if and only if $\mathcal{F}$ and $\mathcal{G}$ are *Holant-indistinguishable*. As #CSP is a special case of Holant, the result of [34] implies the main result Theorem 8 of this work for $\mathbb{F} = \mathbb{R}$. The proof in [34] follows the high-level structure of our intertwiner proof in Section 3, but with several constructions and results, including the automorphism group $\mathrm{Aut}(\mathcal{F})$, its intertwiner space $C_{\mathrm{Aut}(\mathcal{F})}$, and the decomposition of a signature grid into building-block gadgets and the resulting combinatorial characterization of $C_{\mathrm{Aut}(\mathcal{F})}$ (Theorem 21), relaxed from permutations and #CSP to orthogonal transformations and Holant.

Our results Extending the notion of homomorphism-indistinguishablity, say $\mathcal{F}$ and $\mathcal{G}$ are *#CSP-indistinguishable* if the partition function value of every #CSP($\mathcal{F}$) instance is preserved when we replace every constraint function in $\mathcal{F}$ with the corresponding function in $\mathcal{G}$. The main result of this work is the following theorem.

Theorem (Theorem 8, informal). For a field $\mathbb{F}$ of characteristic 0, sets $\mathcal{F}$ and $\mathcal{G}$ of $\mathbb{F}$-valued constraint functions are isomorphic if and only if $\mathcal{F}$ and $\mathcal{G}$ are #CSP-indistinguishable.

Bulatov et al. [4, Theorem 4 and Remark 5] show that the problem of computing the partition function of a #CSP($\mathcal{F}$) instance reduces to computing the partition function of a (much larger) #CSP($\mathcal{F}'$) instance, where $\mathcal{F}'$ is a set of binary (arity-2) constraint functions. This reduction is isomorphism-preserving – that is, if $\mathcal{F} \cong \mathcal{G}$, then the corresponding binary $\mathcal{F}' \cong \mathcal{G}'$. Hence, to prove Theorem 8 it suffices to extend Cai and Govorov's homomorphism indistinguishability theorem from a single binary constraint function (i.e. graph homomorphism) to a set of binary constraint functions. However, hypothetical proofs of an indistinguishability theorem for a set of binary constraint functions would extend quite naturally to the interpolation proof presented below for a set of arbitrary-arity constraint functions. Furthermore, the #CSP instances constructed by our proof are much smaller, simpler and more uniform than those produced by the reduction in [4], which is important because these #CSP instances serve as witnesses for constraint function nonisomorphism, and can be enumerated to make complexity dichotomies *effective* (see below). Thus we choose to use our interpolation technique to tackle the arbitrary-arity case directly.

We prove Theorem 8 in the intertwiner space style of Mančinska and Roberson [28] in Section 3 (for $\mathbb{F} = \mathbb{C}$), and in the Vandermonde interpolation style of Cai and Govorov [12] in Section 4. The two proofs have distinct advantages. The intertwiner proof has a short, clean, combinatorial presentation that avoids the detailed notation of interpolation and the technical graph algebra calculations of [19, 26, 27, 31, 21], while proving generalizations, such as Theorem 21, of the latter group's intermediate results. It also makes no distinction between finite and infinite constraint function sets (interpolation only directly applies to finite sets, but we use the fact that the space of possible isomorphisms is finite to extend the interpolation proof to sets of arbitrary cardinality in Theorem 34) and demonstrates a natural application of the powerful representation-theoretic tools of intertwiner spaces and Tannaka-Krein duality to #CSP and Holant theory; as noted above, Young [34] later used relaxed versions of these tools to prove an indistinguishability theorem for general Holant, a setting which does not admit Vandermonde interpolation.

On the other hand, the interpolation proof, in addition to supporting any field of characteristic zero, actually proves a more general result (Theorem 34) applying to k-labeled #CSP instances. It is also *constructive* (see Section 4.5): if $\mathcal{F}$ and $\mathcal{G}$ are finite and not isomorphic, then the proof provides a finite, explicit list of #CSP instances which must contain an instance on which $\mathcal{F}$ and $\mathcal{G}$ are distinguishable. Cai and Govorov use their constructive interpolation proof to make the graph homomorphism dichotomy of Cai, Chen, and Lu [10] *effective*, meaning there is an algorithm that decides whether the problem is #P-hard (i.e. the dichotomy is decidable) and, if so, constructs a reduction from a #P-hard problem, rather than simply asserting such a reduction exists. Notably, the current complex-weighted #CSP dichotomy [8] is not even known to be decidable; our constructive proof could similarly play a role in a decidable or effective #CSP dichotomy.

2 Preliminaries

For $n \in \mathbb{N}$, write $[n] = \{0, 1, \ldots, n-1\}$. Throughout, we abbreviate tuples $(x_0, \ldots, x_{n-1})$ by boldface letter $\mathbf{x}$. For sets A and B, A^B denotes the set of functions from B to A. For a set B with an implicit linear order and $a_b \in A$ for every $b \in B$, $(a_b)_{b \in B}$ denotes a tuple of elements of A indexed and ordered by B. Let $\mathbb{S}_q$ be the symmetric group of permutations on $[q]$.

Throughout, let $\mathbb{F}$ be a field of characteristic 0. The following simple proposition follows from the fact that a square Vandermonde matrix with distinct rows is always nonsingular.

Proposition 1 ([12, Lemma 4.1])**.** *Let I be a finite index set, and a_i, $b_i \in \mathbb{F}$ for all $i \in I$. Let $I = \bigsqcup_{\ell \in [s]} I_\ell$ be the partition of I into equivalence classes defined by relation $\sim$, where $i \sim i'$ iff $b_i = b_{i'}$. If*

$$\sum_{i \in I} a_i b_i^j = 0$$

for every choice of $j \in [|I|]$, then $\sum_{i \in I_\ell} a_i = 0$ for every $\ell \in [s]$.

2.1 Counting Constraint Satisfaction Problems

Any function $F : V(F)^{n_F} \to \mathbb{F}$ on $n_F \geqslant 1$ variables taking values in $V(F)$ is a *constraint function* with *domain* $V(F)$ and *arity* n_F. When $n_F = 2$, one can view F as a $|V(F)| \times$

$|V(F)|$ matrix with entries in $\mathbb{F}$, the adjacency matrix of an $\mathbb{F}$-*weighted graph* [12]. It is assumed that all constraint functions in a set $\mathcal{F}$ have the same domain, denoted $V(\mathcal{F})$ (V stands for 'vertices', terminology inherited from the weighted graph special case).

Definition 2 (#CSP, $\boldsymbol{Z}$)**.** A *#CSP problem* #CSP($\mathcal{F}$) is parameterized by a set $\mathcal{F}$ of constraint functions. A *#CSP($\mathcal{F}$) instance* $K = (V, C)$ is defined by a set V of variables and a multiset C of *constraints*. Each constraint $(F, v_1, \ldots, v_{n_F})$ consists of a constraint function $F \in \mathcal{F}$ and an ordered tuple of variables to which F is applied.

The *partition function* Z, on input #CSP($\mathcal{F}$) instance $K = (V, C)$, outputs

$$Z(K) = \sum_{\phi: V \to V(\mathcal{F})} \prod_{(F, v_1, \ldots, v_{n_F}) \in C} F(\phi(v_1), \ldots, \phi(v_{n_F})).$$

Definition 3 (Similar, $\boldsymbol{K_{\mathcal{F}\to\mathcal{G}}}$)**.** Constraint function sets $\mathcal{F}$ and $\mathcal{G}$ are *similar* if there is a bijection from $\mathcal{F}$ to $\mathcal{G}$ such that every $F \in \mathcal{F}$ has the same arity as its image $G \in \mathcal{G}$. Call F and its image G *corresponding* constraint functions, denoted $F \leftrightsquigarrow G$.

For similar constraint function sets $\mathcal{F}$ and $\mathcal{G}$ and any #CSP($\mathcal{F}$) instance K, define a #CSP($\mathcal{G}$) instance $K_{\mathcal{F}\to\mathcal{G}}$ by replacing each constraint $(F, v_1, \ldots, v_{n_F})$ of K with $(G, v_1, \ldots, v_{n_F})$, for $G \leftrightsquigarrow F$.

The next definition generalizes k-labeled graphs [19, 26, 12].

Definition 4 ($\boldsymbol{k}$-labeled #CSP instance (product), $\boldsymbol{\mathcal{PLI}[\mathcal{F}; k]}$, $\boldsymbol{\mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; k]}$)**.** A #CSP instance $K = (V, C)$ is *k-labeled* if $|V| \geqslant k$ and k distinct variables are labeled by $[k]$. Define the *product* $K_1 K_2$ of two k-labeled #CSP($\mathcal{F}$) instances $K_1 = (V_1, C_1), K_2 = (V_2, C_2)$ as follows. For $i \in [k]$, let $u_i \in V_1, v_i \in V_2$ be the variables labeled i in V_1 and V_2, respectively. Define a new variable set V by starting with $V_1 \sqcup V_2$, then for each $i \in [k]$ merging u_i and v_i into a new variable w_i, and label w_i by i. Then define a new constraint multiset C by starting with $C_1 \sqcup C_2$ (multiset union), and for every $i \in [k]$ replacing every occurrence of u_i or v_i in each constraint with w_i. Then take $K_1 K_2 = (V, C)$.

Define $\mathcal{PLI}[\mathcal{F}; k]$ to be the set of k-labeled #CSP($\mathcal{F}$) instances. Let $U_k = (V, \varnothing) \in \mathcal{PLI}[\mathcal{F}; k]$, where V contains exactly k variables (all labeled). The k-labeled instance product is commutative and associative and has identity U_k, so $\mathcal{PLI}[\mathcal{F}; k]$ forms a commutative monoid under this product. Let $\mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; k]$ denote the submonoid of $\mathcal{PLI}[\mathcal{F}; k]$ consisting of *simple* instances – those where the variables in any constraint $c \in C$ are distinct and the multiplicity of every constraint in C is 1 up to permutation of the order of its variables.

Definition 5 ($\boldsymbol{Z^{\psi}}$)**.** For $K = (V, C) \in \mathcal{PLI}[\mathcal{F}; k]$ and a map $\psi : [k] \to V(\mathcal{F})$ fixing, or *pinning*, the values of the labeled variables, define

$$Z^{\psi}(K) = \sum_{\phi: V \to V(\mathcal{F}) \text{ extends } \psi} \prod_{(F, v_1, \ldots, v_{n_F}) \in C} F(\phi(v_1), \ldots, \phi(v_{n_F})),$$

where ϕ extends ψ means ϕ assigns value $\psi(i)$ to the variable labeled i.

The k-labeled instance product K_1K_2 merges the labeled variables, and the unlabeled variables of K_1 and K_2 both still appear in constraints from K_1 and K_2. The unlabeled variables of K_1 take values independently of the unlabeled variables of K_2 (i.e. they appear in no constraints with each other). Hence the k-labeled instance product induces an entrywise product on the $Z^{(\cdot)}$ maps:

$$Z^{\psi}(K_1K_2) = Z^{\psi}(K_1)Z^{\psi}(K_2). \tag{2}$$

Definition 6 (#CSP-indistinguishable)**.** For pinning maps $\varphi : [k] \to V(\mathcal{F})$ and $\psi : [k] \to V(\mathcal{G})$, say $(\mathcal{F}, \varphi)$ and $(\mathcal{G}, \psi)$ are *#CSP-indistinguishable* if $Z^{\varphi}(K) = Z^{\psi}(K_{\mathcal{F}\to\mathcal{G}})$ for every $K \in \mathcal{PLI}[\mathcal{F}; k]$.

If $k = 0$, simply say that $\mathcal{F}$ and $\mathcal{G}$ are #CSP-indistinguishable.

Say $(\mathcal{F}, \varphi)$ and $(\mathcal{G}, \psi)$ are *simple-*#CSP*-indistinguishable* if $Z^{\varphi}(K) = Z^{\psi}(K_{\mathcal{F}\to\mathcal{G}})$ for every $K \in \mathcal{PLI}^{\text{simp}}[\mathcal{F}; k]$.

Definition 7 ($\cong$, **Aut**)**.** Let F, G be constraint functions of common arity n and $|V(\mathcal{F})| = |V(\mathcal{G})|$. A bijection $\sigma : V(F) \to V(G)$ is a *isomorphism* from F to G if $F(\mathbf{x}) = G(\sigma(\mathbf{x}))$ for all $\mathbf{x} \in V(F)^n$, where $\sigma(\mathbf{x}) = (\sigma(x_0), \ldots, \sigma(x_{n-1}))$.

Say similar constraint function sets $\mathcal{F}$ and $\mathcal{G}$ are isomorphic ($\mathcal{F} \cong \mathcal{G}$) if there is a single $\sigma : V(\mathcal{F}) \to V(\mathcal{G})$ which is an isomorphism between every pair $\mathcal{F} \ni F \leftrightsquigarrow G \in \mathcal{G}$.

For $\varphi : [k] \to V(\mathcal{F})$ and $\psi : [k] \to V(\mathcal{G})$, say $(\mathcal{F}, \varphi) \cong (\mathcal{G}, \psi)$ if there is an isomorphism $\sigma : V(\mathcal{F}) \to V(\mathcal{G})$ satisfying $\psi = \sigma \circ \varphi$.

Define $\text{Aut}(\mathcal{F})$ to be the group of all isomorphisms from $\mathcal{F}$ to itself.

We emphasize that every corresponding pair of functions in $\mathcal{F}$ and $\mathcal{G}$ must be isomorphic via the same σ. If $\mathcal{F} \cong \mathcal{G}$, then, since an isomorphism is just a relabeling of the domain elements, $\mathcal{F}$ and $\mathcal{G}$ are #CSP-indistinguishable. Our main theorem is the converse of this fact, a generalization of the fact that graphs $X \cong Y$ iff X and Y are homomorphism-indistinguishable:

Theorem 8. *Let $\mathbb{F}$ be a field of characteristic 0, and let $\mathcal{F}$ and $\mathcal{G}$ be similar $\mathbb{F}$-valued constraint function sets. Then $\mathcal{F} \cong \mathcal{G}$ if and only if $\mathcal{F}$ and $\mathcal{G}$ are* #CSP*-indistinguishable.*

3 The Intertwiner Proof

In this section, we prove Theorem 8 for $\mathbb{F} = \mathbb{C}$.

The following construction 'flattens' a constraint function into a matrix.

Definition 9 ($\boldsymbol{F^{m,d}}$, $\boldsymbol{f}$)**.** For an n-ary constraint function $F \in \mathbb{F}^{[q]^n}$ on domain $[q]$ and any $m, d \geqslant 0, m + d = n$, define the matrix $F^{m,d} \in \mathbb{F}^{q^m \times q^d}$ by

$$(F^{m,d})_{\mathbf{x},\mathbf{y}} = F(x_0, \ldots, x_{m-1}, y_{d-1}, \ldots, y_0)$$

for $\mathbf{x} \in [q]^m$ and $\mathbf{y} \in [q]^d$ (and using the standard bijection between $[q^m]$ and $[q]^m$).

Abbreviate $f := F^{n,0} \in \mathbb{F}^{q^n}$, called the *signature vector* of F.

Note that the bits of the column index of $F^{m,d}$ are reversed. This is done so that the definition matches Definition 11 of a gadget signature matrix below.

3.1 Holant Problems and Gadgets

The proof is carried out in the Holant framework, a generalization of #CSP. See the book by Cai and Chen [7] for an introduction to Holant theory. Like a #CSP problem, a Holant problem Holant($\mathcal{F}$) is is parameterized by a set $\mathcal{F}$ of constraint functions, called *signature functions* or *signatures*. The input to Holant($\mathcal{F}$) is a *signature grid* Ω, which consists of an underlying multigraph with vertex set V and edge set E, along with an assignment of a signature $F_v \in \mathcal{F}$ to each vertex $v \in V$, where F_v has arity $\deg(v)$. The edges $E(v)$ incident to v are given an order and serve as the input variables to F_v, taking values in $V(\mathcal{F})$. The output on input Ω is

$$\mathrm{Holant}_\Omega(\mathcal{F}) = \sum_{\sigma: E \to V(\mathcal{F})} \prod_{v \in V} F_v(\sigma|_{E(v)}), \tag{3}$$

where $F_v(\sigma|_{E(v)})$ is the evaluation of F_v on the ordered tuple $\sigma|_{E(v)}$, the restriction of σ to $E(v)$. For example, consider the signature set $\mathcal{EO} = \{\mathrm{EO}_n \mid n \geqslant 1\}$ with $V(\mathcal{EO}) = [2] = \{0, 1\}$, and EO_n is the n-ary signature taking value 1 when exactly one of its inputs is 1 (and the rest are 0), and taking value 0 otherwise. Then $\mathrm{Holant}_\Omega(\mathcal{EO})$ counts the number of perfect matchings in the underlying multigraph of Ω. For another example, consider the signature set $\mathcal{NEQ} = \{\neq_n \mid n \geqslant 1\}$ on domain $V(\mathcal{NEQ}) = [q]$, where $\neq_n$ is the n-ary signature taking value 1 when its n inputs are distinct, and 0 otherwise. Then $\mathrm{Holant}_\Omega(\mathcal{NEQ})$ counts the number of proper edge-q-colorings of Ω.

For sets $\mathcal{F}$ and $\mathcal{G}$ of signatures define the problem Holant($\mathcal{F} \mid \mathcal{G}$), which takes as input a signature grid with a bipartite underlying multigraph with bipartition $V = V_1 \cup V_2$ such that the vertices in V_1 and V_2 are assigned signatures from $\mathcal{F}$ and $\mathcal{G}$, respectively.

Definition 10 (**$E_n, E^{m,d}$, $\mathcal{EQ}$**)**.** Define the n-ary *equality* constraint function $E_n \in \{0,1\}^{[q]^n}$ by $E_n(x_1, \ldots, x_n) = 1$ if $x_1 = \ldots = x_n$, and 0 otherwise, for $x_1, \ldots, x_n \in [q]$ (we suppress the dependence on q, which will be clear from context). Write $E^{m,d} := (E_n)^{m,d}$, as we must have $m + d = n$. Define $\mathcal{EQ} = \{E_n \mid n \geqslant 1\}$.

Let $\mathcal{F}$ be a set of constraint functions. To each #CSP($\mathcal{F}$) instance $K = (V, C)$ we associate a biparite signature grid Ω_K in the context of Holant($\mathcal{F} \mid \mathcal{EQ}$), constructed as follows. For each variable $v \in V$, create a vertex u_v – called an *equality vertex* – assigned E_{n_v}, where n_v is the total number of appearances of v in the constraints in C. Then, for every constraint $c = (F, v_1, \ldots, v_{n_F}) \in C$, create a vertex w_c assigned F, called a *constraint vertex*, adjacent to the equality vertices $u_{v_1}, \ldots, u_{v_{n_F}}$ (ordering the edges incident to w_c accordingly). Any edge assignment σ must assign all edges incident to an equality vertex the same value (or else the term corresponding to σ is 0), so we can view σ as #CSP variable assignment. Hence $Z(K) = \mathrm{Holant}_{\Omega_K}(\mathcal{F} \mid \mathcal{EQ})$.

Definition 11 (Gadget, **M(K)**, **$\mathfrak{G}_{\mathcal{F}}(m,d)$**, **$\mathfrak{G}_{\mathcal{F}}$**)**.** A *gadget* is a Holant signature grid equipped with an ordered set of dangling edges (edges with only one endpoint), defining external variables. Let $\mathfrak{G}_{\mathcal{F}}(m,d)$ be the collection of all gadgets in the context of Holant($\mathcal{F} \mid \mathcal{EQ}$) with m *left* dangling edges $\ell_0, \ldots, \ell_{m-1}$ and d *right* dangling edges

$r_0, \ldots, r_{d-1}$, drawn on the left and right of the gadget, respectively, from top to bottom. We assume all dangling edges are incident to equality vertices. Let $\mathfrak{G}_{\mathcal{F}} = \bigcup_{m,d} \mathfrak{G}_{\mathcal{F}}(m,d)$.

For $\mathbf{K} \in \mathfrak{G}_{\mathcal{F}}(m,d)$, with $V(\mathcal{F}) = [q]$, define the *signature matrix* $M(\mathbf{K}) \in \mathbb{C}^{q^m \times q^d}$ of $\mathbf{K}$ by, for $\mathbf{x} \in [q]^m$ and $\mathbf{y} \in [q]^d$, letting $M(\mathbf{K})_{\mathbf{x},\mathbf{y}}$ be the Holant value of $\mathbf{K}$ when its m left and d right dangling edges are fixed to $x_0, \ldots, x_{m-1} \in [q]$ and $y_0, \ldots, y_{d-1} \in [q]$, respectively.

Definition 12 (Gadget $\circ, \otimes, \dagger$)**.** Define the following operations on gadgets (see Figure 1).

- Given $\mathbf{K} \in \mathfrak{G}_{\mathcal{F}}(j,m), \mathbf{L} \in \mathfrak{G}_{\mathcal{F}}(m,d)$, construct $\mathbf{K} \circ \mathbf{L} \in \mathfrak{G}_{\mathcal{F}}(j,d)$ by placing $\mathbf{L}$ to the right of $\mathbf{K}$, and merging the ith right dangling edge of $\mathbf{K}$ with the ith left dangling edge of $\mathbf{L}$, for $i \in [m]$. If composition makes vertices assigned $E_a, E_b \in \mathcal{EQ}$ adjacent, contract the edge between them and assign the resulting merged vertex E_{a+b-2} (to preserve bipartiteness). This does not change the Holant value.

- For gadgets $\mathbf{K} \in \mathfrak{G}_{\mathcal{F}}(m_1,d_1), \mathbf{L} \in \mathfrak{G}_{\mathcal{F}}(m_2,d_2)$, construct $\mathbf{K} \otimes \mathbf{L} \in \mathfrak{G}_{\mathcal{F}}(m_1+m_2, d_1+d_2)$ by taking the disjoint union of the multigraphs underlying $\mathbf{K}$ and $\mathbf{L}$, placing $\mathbf{K}$ above $\mathbf{L}$.

- For $\mathbf{K} \in \mathfrak{G}_{\mathcal{F}}(m,d)$, construct $\mathbf{K}^\dagger \in \mathfrak{G}_{\overline{\mathcal{F}}}(d,m)$ by reflecting the underlying multigraph of $\mathbf{K}$ horizontally, and replacing every signature F with its entrywise conjugate $\overline{F}$.

It is well known (see e.g. [7, Section 1.3]) that $M(\mathbf{K}_1 \circ \mathbf{K}_2) = M(\mathbf{K}_1) \circ M(\mathbf{K}_2)$, $M(\mathbf{K}_1 \otimes \mathbf{K}_2) = M(\mathbf{K}_1) \otimes M(\mathbf{K}_2)$, and $M(\mathbf{K}^\dagger) = M(\mathbf{K})^\dagger$ – that is, the gadget operations $\circ, \otimes, \dagger$ induce the matrix operations composition, Kronecker product, and conjugate transpose, respectively.

An $(m+d)$-labeled #CSP($\mathcal{F}$) instance $K \in \mathcal{PLI}[\mathcal{F}; m+d]$ corresponds to a gadget $\mathbf{K} \in \mathcal{G}_{\mathcal{F}}(m,d)$ with dangling edges incident to the equality vertices constructed from the labeled variables. For a map $\psi : [m+d] \to V(\mathcal{F})$ assigning values $x_0, \ldots, x_{m-1}, y_0, \ldots, y_{d-1} \in V(\mathcal{F})$ to the labeled variables, we have $M(\mathbf{K})_{\mathbf{x},\mathbf{y}} = Z^\psi(K)$, because giving an equality vertex input x along a dangling edge forces its incident edges to take value x, pinning the corresponding variable to x.

Definition 13 ($\mathbf{E}^{m,d}, \mathbf{I}, \mathbb{F}$)**.** For $m, d \geqslant 0$, let $\mathbf{E}^{m,d}$ be the gadget consisting of a single vertex, assigned E_{m+d}, with m left and d right dangling edges. Define $\mathbf{I} := \mathbf{E}^{1,1}$.

For an n-ary signature F, let $\mathbb{F}$ be the gadget consisting of a degree-n vertex assigned F, adjacent to n degree-2 vertices assigned E_2, each of which is incident to a left dangling edge. See Figure 2 for illustrations.

Ignoring (i.e. treating as edges) vertices assigned E_2 has no effect on the Holant value. In particular, the ith input to the gadget $\mathbb{F}$ equals the ith input to the signature F, so

$$M(\mathbf{E}^{m,d}) = E^{m,d} \text{ and } M(\mathbb{F}) = f$$

(recall that $f = F^{n_F,0}$ is the signature vector of F). If we pivot the last d left dangling edges of $\mathbb{F}$ to the right, preserving their cyclic order around the central vertex, the resulting

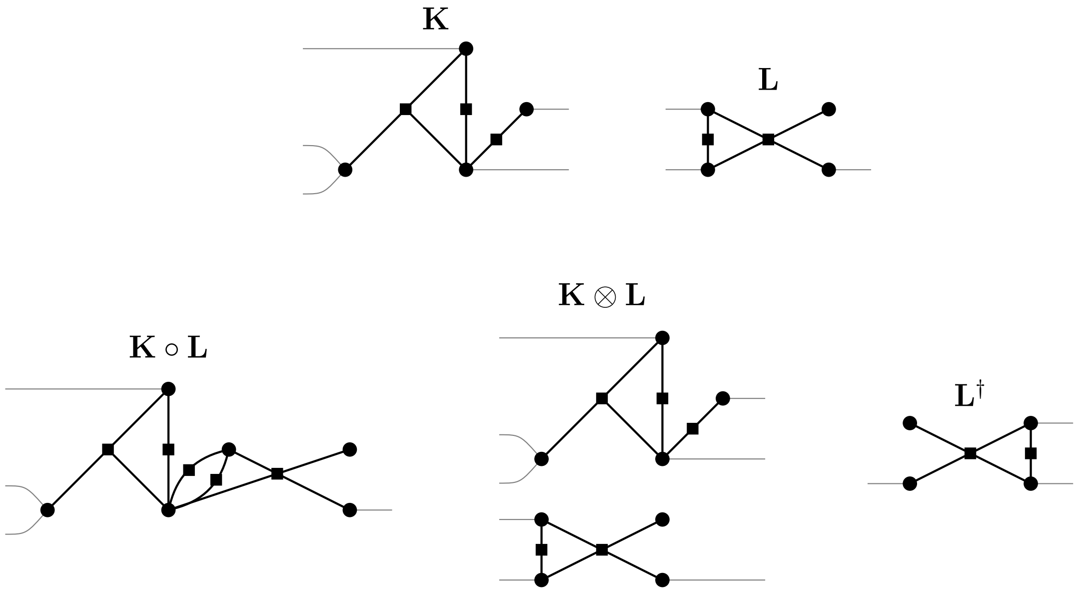

Figure 1: Gadgets $\mathbf{K} \in \mathfrak{G}_{\mathcal{F}}(3,2)$ and $\mathbf{L} \in \mathfrak{G}_{\mathcal{F}}(2,1)$, and their composition $\mathbf{K}\circ\mathbf{L} \in \mathfrak{G}_{\mathcal{F}}(3,1)$, tensor product $\mathbf{K}\otimes\mathbf{L} \in \mathfrak{G}_{\mathcal{F}}(5,3)$, and transpose $\mathbf{L}^\dagger \in \mathfrak{G}_{\mathcal{F}}(1,2)$. Equality and constraint vertices are drawn as circles and squares, respectively.

gadget in $\mathfrak{G}_{\mathcal{F}}(n_F - d, d)$ has signature matrix $F^{n_F-d,d}$ (this is the purpose of reversing the right indices in Definition 9, as the top-down order of the d pivoted edges is reversed).

Definition 14 ($\mathbf{S}_{\boldsymbol{\sigma}}$, $\mathbf{S}$, $\boldsymbol{S}$)**.** For permutation $\sigma \in \mathbb{S}_k$, let $\mathbf{S}_\sigma \in \mathfrak{G}(k,k)$ be the gadget formed from $\mathbf{I}^{\otimes k}$ by permuting the dangling ends of the right dangling edges according to σ – that is, the ith left dangling edge is incident to the same E_2 vertex as the $\sigma(i)$th right dangling edge (see Figure 3). Given left inputs $\mathbf{x} \in [q]^k$ and right inputs $\mathbf{y} \in [q]^k$, $\mathbf{S}_\sigma$ evaluates to evaluates to 1 if $x_i = y_{\sigma(i)}$ for all $i \in [k]$, and evaluates to 0 otherwise.

Abbreviate $\mathbf{S} := \mathbf{S}_{(1\ 2)}$ and let S be the 4-ary signature of $\mathbf{S}$ (so $S^{2,2} = M(\mathbf{S})$). See Figure 2.

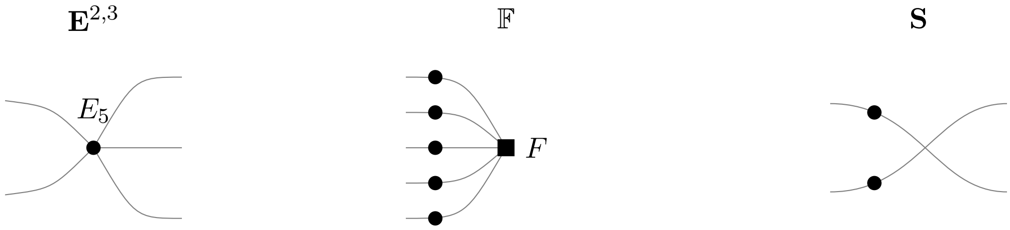

Figure 2: Basic gadgets $\mathbf{E}^{2,3}$, $\mathbb{F}$ (for 5-ary F), and $\mathbf{S}$.

We will compose $\mathbf{S}_\sigma$ with other gadgets to permute their dangling edges. As noted above, ignoring E_2 vertices does not affect the Holant value; hence we can view $\mathbf{S}_\sigma$ as a gadget composed solely of two-sided dangling edges. Analogously to generating the braid group by crossing adjacent strands, we can construct any $\mathbf{S}_\sigma$ using only $\mathbf{I}$ and $\mathbf{S}$. Let $\langle \mathcal{M} \rangle_{\circ,\otimes,\dagger}$ denote the closure of a set $\mathcal{M}$ of gadgets or signature matrices under $\circ, \otimes, \dagger$.

Proposition 15. *For any $k \geqslant 2$ and $\sigma \in \mathbb{S}_k$, we have $\mathbf{S}_\sigma \in \langle \mathbf{I}, \mathbf{S} \rangle_{\circ,\otimes,\dagger}$.*

Proof. Decompose σ into adjacent transpositions as $\sigma = (a_1\ a_1{+}1)(a_2\ a_2{+}1)\dots(a_s\ a_s{+}1)$. Then, since $\mathbf{S}$ swaps the position of adjacent dangling edges, we have (see Figure 3)

$$\mathbf{S}_\sigma = \bigcirc_{i=1}^{s} (\mathbf{I}^{\otimes a_i - 1} \otimes \mathbf{S} \otimes \mathbf{I}^{\otimes k - a_i - 1}). \qquad \square$$

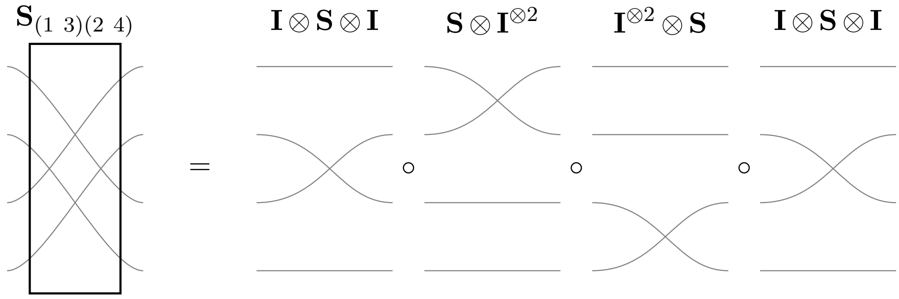

Figure 3: Illustrating the decomposition of $\mathbf{S}_\sigma$ given by Proposition 15, with $\sigma = (1\ 3)(2\ 4) = (2\ 3)(1\ 2)(3\ 4)(2\ 3)$.

The next theorem is an extension of [28, Theorem 8.4] from the setting of unweighted graph homomorphism (where $\mathcal{F}$ contains a single binary symmetric 0-1 valued constraint function) to any set of real-valued constraint functions.

Theorem 16. *For any $\mathbb{R}$-valued constraint function set $\mathcal{F}$,*

$$\mathfrak{G}_{\mathcal{F}} = \langle \mathbf{E}^{1,0}, \mathbf{E}^{1,2}, \mathbf{S}, \{\mathbb{F} \mid F \in \mathcal{F}\} \rangle_{\circ,\otimes,\dagger}.$$

If $\mathcal{F}$ is $\mathbb{C}$-valued, then $\mathfrak{G}_{\mathcal{F}} \subset \langle \mathbf{E}^{1,0}, \mathbf{E}^{1,2}, \mathbf{S}, \{\mathbb{F} \mid F \in \mathcal{F}\} \rangle_{\circ,\otimes,\dagger}$.

Proof. Observe that $\mathfrak{G}_{\mathcal{F}}$ is closed under $\otimes$ and, for real-valued $\mathcal{F}$, under $\dagger$. By definition, all dangling edges of gadgets in $\mathcal{F}$ are incident to equality vertices, and $\circ$ preserves bipartiteness by contracting the edges between adjacent equality vertices. Therefore $\mathfrak{G}_{\mathcal{F}}$ is also closed under $\circ$, giving the $\supset$ inclusion. To show the $\subset$ inclusion, first observe that by chaining copies of $\mathbf{E}^{1,2}$, we can construct any $\mathbf{E}^{m,d}$. Formally, $\mathbf{I} = \mathbf{E}^{1,2} \circ (\mathbf{E}^{1,2})^\dagger$,

$$\mathbf{E}^{m,d} = \bigcirc_{i=0}^{m-2} (\mathbf{E}^{2,1} \otimes \mathbf{I}^{\otimes i}) \circ \bigcirc_{i=0}^{d-2} (\mathbf{E}^{1,2} \otimes \mathbf{I}^{\otimes i})$$

for any $m, d \geqslant 2$, and $\mathbf{E}^{m,d} = \mathbf{E}^{m,1} \circ \bigcirc_{i=0}^{d-2} (\mathbf{E}^{1,2} \otimes \mathbf{I}^{\otimes i})$ for $m \in \{0, 1\}$, $d \geqslant 2$. Also $\mathbf{E}^{0,0} = \mathbf{E}^{0,1} \circ \mathbf{E}^{1,0}$. Thus we obtain the following recontextualization of [28, Lemma 3.18]):

$$\mathbf{E}^{m,d} \in \langle \mathbf{E}^{1,2}, \mathbf{E}^{1,0} \rangle_{\circ,\otimes,\dagger} \text{ for all } m, d \geqslant 0. \tag{4}$$

Consider a Holant($\mathcal{F} \mid \mathcal{EQ}$) gadget $\mathbf{K} \in \mathfrak{G}_\mathcal{F}(M, D)$. We will construct $\mathbf{K}$ from the basic gadgets (see Figure 4). Suppose $\mathbf{K}$ contains r equality vertices, which we denote $e_1, \ldots, e_r$ in arbitrary order, and s constraint vertices, denoted $c_1, \ldots, c_s$ in arbitrary order, with c_j assigned signature $F_j \in \mathcal{F}$. For $i \in [r]$, suppose vertex e_i is incident to m_i left and d_i right dangling edges in $\mathbf{K}$, respectively, and has degree $m_i + d_i + t_i$. Let $T = \sum_{i=1}^r t_i = \sum_{j=1}^s \deg(c_j)$. We also have $M = \sum_{i=1}^r m_i$ and $D = \sum_{i=1}^r d_i$, because by assumption all dangling edges are incident to equality vertices. Let $\mathbf{K}_0 = \bigotimes_{i=1}^r \mathbf{E}^{m_i, d_i+t_i} \in \mathfrak{G}_\mathcal{F}(M, D+T)$ and identify e_i with the vertex in $\mathbf{E}^{m_i, d_i+t_i}$. By the bipartite structure of $\mathbf{K}$, for all $k \in [\text{arity}(F_1)] = [\deg(c_1)]$, the kth input to c_1 is incident to some equality vertex e_{i_k}. Identifying c_1 with the vertex in $\mathbb{F}_1$ (and inserting the dummy E_2 vertices), there is a permutation $\sigma_1 \in \mathbb{S}_{D+T}$ such that, in the gadget

$$\mathbf{K}_1 = \mathbf{K}_0 \circ \mathbf{S}_{\sigma_1} \circ (\mathbb{F}_1 \otimes \mathbf{I}^{\otimes D+T-\text{arity}(F_1)}) \in \mathfrak{G}_\mathcal{F}(M, D+T-\text{arity}(F_1)),$$

the kth input to c_1 is merged with the proper edge incident to e_{i_k} for every $k \in [\text{arity}(F_1)]$. Similarly, for each $j \in [s]$, let $\sigma_j \in \mathbb{S}_{D+T-\sum_{\ell=1}^{j-1} \text{arity}(F_\ell)}$ be the permutation that matches c_j's incident edges with the proper equality vertices. Then

$$\mathbf{K}_s = \mathbf{K}_0 \circ \bigcirc_{j=1}^s \left(\mathbf{S}_{\sigma_j} \circ \left(\mathbb{F}_j \otimes \mathbf{I}^{\otimes D+T-\sum_{\ell=1}^{j} \text{arity}(F_\ell)} \right) \right) \in \mathfrak{G}_\mathcal{F}(M, D),$$

is a gadget with the same internal structure as $\mathbf{K}$. Finally, there exist $\tau \in S_M$ and $\upsilon \in S_D$ that order the left and right dangling edges properly: $\mathbf{K} = \mathbf{S}_\tau \circ \mathbf{K}_s \circ \mathbf{S}_\upsilon$. By Proposition 15 and (4), $\mathbf{K} \in \langle \mathbf{E}^{1,0}, \mathbf{E}^{1,2}, \mathbf{S}, \{\mathbb{F} \mid F \in \mathcal{F}\} \rangle_{\circ,\otimes,\dagger}$. $\square$

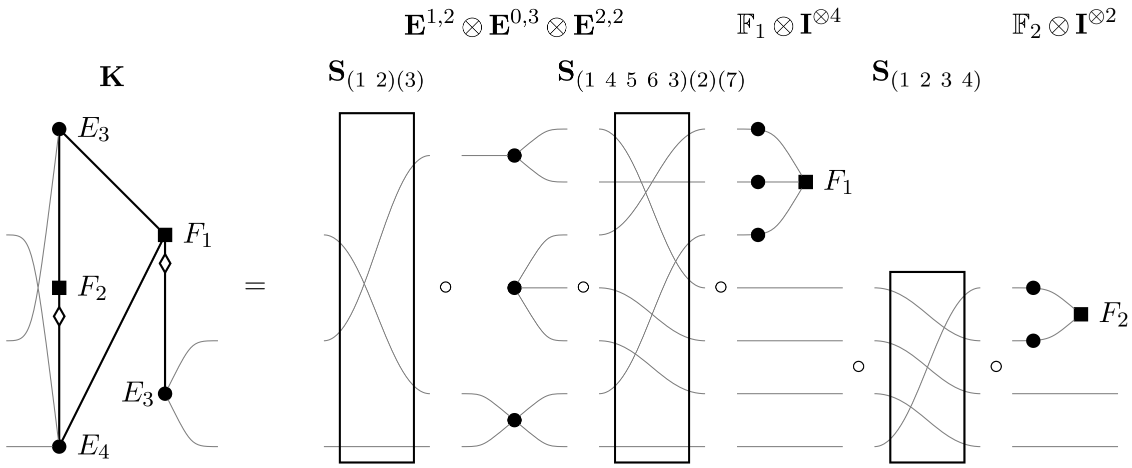

Figure 4: Illustrating the Theorem 16 decomposition of a $\mathbf{K} \in \mathfrak{G}(3, 2)$. We draw dangling edges thinner than internal edges, and use circles for equality vertices and squares for constraint vertices. A diamond on an edge marks this edge as the first input to the incident constraint vertex, and inputs proceed counterclockwise.

The $\supset$ inclusion of Theorem 16 does not hold for complex-valued $\mathcal{F}$, because such $\mathcal{F}$ are in general not closed under entrywise conjugation, a by-product of the $\dagger$ operator.

However, the real-valued case suffices to prove the below Theorem 21 even for complex-valued $\mathcal{F}$.

3.2 Intertwiner Spaces

Let H be a subgroup of the group $\mathbb{O}_q$ of (real) $q \times q$ orthogonal matrices. The (m,d)-*intertwiner space* of H is

$$C_H(m,d) = \{M \in \mathbb{C}^{q^m} \times \mathbb{C}^{q^d} \mid \forall A \in H : A^{\otimes m} M = M A^{\otimes d}\}.$$

Define $C_H = \bigcup_{m,d} C_H(m,d)$ to be the set of all intertwiners of H.

We will identify $\sigma \in \mathbb{S}_q$ with the associated permutation matrix $P_\sigma \in \{0,1\}^{q \times q}$. With this perspective, we consider subgroups $H \subset \mathbb{S}_q \subset \mathbb{O}_q$. If P_σ is a $q \times q$ permutation matrix, then, for a vector $\mathbf{v} \in \mathbb{C}^{q^n} \cong \mathbb{C}^{[q]^n}$, $P_\sigma^{\otimes n}\mathbf{v}$ is the vector obtained by permuting the entries of $\mathbf{v}$ according to the natural action of σ on $[q]^n \cong [q^n]$ – that is, for $\mathbf{x} \in [q]^n$,

$$(P_\sigma^{\otimes n}\mathbf{v})_{\mathbf{x}} = v_{\sigma(\mathbf{x})} = v_{(\sigma(x_1),\ldots,\sigma(x_n))}.$$

Hence, if $\mathbf{x}, \mathbf{y} \in [q]^n$ are in the same orbit of the action of H, then every $(n,0)$-intertwiner takes equal values on $\mathbf{x}$ and $\mathbf{y}$. Conversely, if $\mathbf{x}, \mathbf{y}$ are not in the same orbit, then the $(n,0)$ intertwiner which is 1 on the orbit containing $\mathbf{x}$ and 0 elsewhere separates $\mathbf{x}$ and $\mathbf{y}$. Therefore we have

Proposition 17. *Let $H \subset \mathbb{S}_q$. Then*

$$v_{\mathbf{x}} = v_{\mathbf{y}} \textit{ for every } \mathbf{v} \in C_H(n,0) \textit{ if and only if there exists a } \sigma \in H \textit{ such that } \sigma(\mathbf{x}) = \mathbf{y}\,.$$

It is well-known (see e.g. [1, Proposition 1.2]) – and can be verified directly – that for any $H \subset \mathbb{O}_q$, C_H is a *symmetric tensor category with duals*, meaning each $C_H(m,d)$ is a vector space over $\mathbb{C}$ and C_H is closed under $\circ, \otimes, \dagger$ and satisfies $I = E^{1,1} \in C_H(1,1)$, $E^{2,0} \in C_H(2,0)$, and $S^{2,2} \in C_H(2,2)$.

The next theorem is a classical version of Woronowicz's Tannaka-Krein duality [32], expressed in this form by Banica and Speicher [1, Theorem 1.3]. It is the key result underlying our first proof of Theorem 8.

Theorem 18. *The mapping $H \mapsto C_H$ induces an inclusion-reversing bijection between (compact) subgroups $H \subset \mathbb{O}_q$ and symmetric tensor categories with duals.*

Let $\langle \mathcal{M} \rangle_{+,\circ,\otimes,\dagger}$ denote the closure of a set $\mathcal{M}$ of signature matrices under $\circ, \otimes, \dagger$, and $\mathbb{C}$-linear combinations of matrices with matching dimensions. The following well-known result, stated in this form by Chassaniol [14], characterizes the intertwiners of $\mathbb{S}_q$.

Proposition 19. $C_{\mathbb{S}_q} = \langle E^{1,0}, E^{1,2}, S^{2,2} \rangle_{+,\circ,\otimes,\dagger}$.

Proof. First observe that $\langle E^{1,0}, E^{1,2}, S^{2,2} \rangle_{+,\circ,\otimes,\dagger}$ is a symmetric tensor category with duals (it contains $E^{1,1}$ and $E^{2,0}$ by the proof of Theorem 16). Hence, by Theorem 18, $\langle E^{1,0}, E^{1,2}, S^{2,2} \rangle_{+,\circ,\otimes,\dagger} = C_H$ for some $H \subset \mathbb{O}_q$. It follows from direct calculation that a matrix $A \in \mathbb{C}^{q\times q}$ satisfies $AE^{1,0} = E^{1,0}$ and $E^{0,1} = E^{0,1}A$ iff every row and column of A sums to 1 ($E^{1,0}$ and $E^{0,1} = (E^{1,0})^\dagger$ are all-ones column and row vectors), and $A^{\otimes 2}E^{2,1} = E^{2,1}A$ and $AE^{1,2} = E^{1,2}A^{\otimes 2}$ iff the products of distinct entries in the same row or column of A is 0. These conditions are equivalent to A being a permutation matrix. Thus $E^{1,0}, E^{1,2} \in C_{\mathbb{S}_q}$, so $\langle E^{1,0}, E^{1,2}, S^{2,2}\rangle_{+,\circ,\otimes,\dagger} \subset C_{\mathbb{S}_q}$, and every $A \in H$ is a permutation matrix, so $H \subset \mathbb{S}_q$, which implies $\langle E^{1,0}, E^{1,2}, S^{2,2}\rangle_{+,\circ,\otimes,\dagger} = C_H \supset C_{\mathbb{S}_q}$. □

Banica and Speicher [1, Theorem 1.10] classify $C_{\mathbb{S}_q}$ as the set of linear combinations of matrices of *partition categories*, or, in our terminology, signature matrices of $\mathfrak{G}_\varnothing$ gadgets (gadgets composed of only signatures in $\mathcal{EQ}$). Using this characterization, Proposition 19 also follows directly from Theorem 16 with $\mathcal{F} = \varnothing$. The next lemma generalizes Proposition 19 to nonempty $\mathcal{F}$. It is an extension of [14, Proposition 3.5] from graphs to arbitrary complex-valued signature sets. Assume $V(\mathcal{F}) = [q]$, so $\mathrm{Aut}(\mathcal{F}) \subset \mathbb{S}_q$.

Lemma 20. $C_{\mathrm{Aut}(\mathcal{F})} = \langle E^{1,0}, E^{1,2}, S^{2,2}, \{f \mid F \in \mathcal{F}\}\rangle_{+,\circ,\otimes,\dagger}$.

Proof. By Proposition 19, $\langle E^{1,0}, E^{1,2}, S^{2,2}, \{f \mid F \in \mathcal{F}\}\rangle_{+,\circ,\otimes,\dagger} \supset C_{\mathbb{S}_q}$, so, by Theorem 18, $\langle E^{1,0}, E^{1,2}, S^{2,2}, \{f \mid F \in \mathcal{F}\}\rangle_{+,\circ,\otimes,\dagger} = C_H$ for some $H \subset \mathbb{S}_q$. By definition, $\sigma \in \mathrm{Aut}(\mathcal{F})$ if and only if $P_\sigma^{\otimes \operatorname{arity}(F)} f = f$ for every $F \in \mathcal{F}$. Therefore each $f \in C_{\mathrm{Aut}(\mathcal{F})}(\operatorname{arity}(F), 0)$, so $C_H \subset C_{\mathrm{Aut}(\mathcal{F})}$, and $H \subset \mathrm{Aut}(\mathcal{F})$, so $C_H \supset C_{\mathrm{Aut}(\mathcal{F})}$. □

Define an (m,d)-*quantum* $\mathcal{F}$-*gadget* to be a formal $\mathbb{C}$-linear combination of gadgets in $\mathfrak{G}_{\mathcal{F}}(m,d)$. In the context of counting homomorphisms to graph X (equivalently, #CSP($\{A_X\}$)), an (m,d)-quantum $\{A_X\}$-gadget is equivalent to an $(m+d)$-*labeled quantum graph* [19, 26, 27]. Let $\mathfrak{Q}_{\mathcal{F}}(m,d)$ be the set of all (m,d)-quantum $\mathcal{F}$-gadgets. Extend the signature matrix function M linearly to $\mathfrak{Q}_{\mathcal{F}}(m,d)$. Observe that, for a fixed (m,d), the set on the RHS of Theorem 20 is the span of the signature matrices of the gadgets in the set on the RHS of Theorem 16. Therefore

$$C_{\mathrm{Aut}(\mathcal{F})}(m,d) = \{M(\mathbf{Q}) \mid \mathbf{Q} \in \mathfrak{Q}_{\mathcal{F}}(m,d)\} \text{ for any set } \mathcal{F} \text{ of } \mathbb{R}\text{-valued constraint functions.} \tag{5}$$

Since equality in Theorem 16 only holds for $\mathbb{R}$-valued $\mathcal{F}$, we do not immediately obtain (5) for $\mathbb{C}$-valued $\mathcal{F}$. However, the #CSP setting admits, via the k-labeled instance product, the construction of arbitrary entrywise products of signatures (recall (2)), which, as we will see again in Section 4, enables Vandermonde interpolation (see also [24, Lemma 2.3]). Here, we use interpolation to extend (5) to the complex-valued case, as in the proof of [13, Lemma 19] (credited to an anonymous reviewer). This technique only applies to sets of binary constraint functions in the planar setting of [13], but here violating planarity is not an issue.

Theorem 21. $C_{\mathrm{Aut}(\mathcal{F})}(m,d) = \{M(\mathbf{Q}) \mid \mathbf{Q} \in \mathfrak{Q}_{\mathcal{F}}(m,d)\}$ *for any set* $\mathcal{F}$ *of* $\mathbb{C}$-*valued constraint functions.*

Proof. Let $F \in \mathcal{F} \cap \mathbb{C}^{[q]^n}$. For $i \geqslant 0$, construct an n-labeled #CSP(F) instance K^i consisting of n labeled variables $v_0, \ldots, v_{n-1}$ and i copies of the constraint $(F, v_0, \ldots, v_{n-1})$.

Let $\mathbf{K}^i \in \mathfrak{G}_{\mathcal{F}}(n,0)$ be the corresponding n-ary gadget. Then $M(\mathbf{K}^i) = f^{\bullet i}$, the ith entry-wise power of the signature vector $f \in \mathbb{C}^{q^n}$ of F (and $f^{\bullet 0}$ is the all-ones vector). Choose p rows of the matrix $\begin{bmatrix} f^{\bullet 0} & f^{\bullet 1} & \dots & f^{\bullet p-1} \end{bmatrix}$ whose second entries are the p distinct entries $b_0, \dots, b_{p-1}$ of f. If some linear combination of these rows with coefficients $a_0, \dots, a_{p-1}$ equals zero, then, by Proposition 1, each $a_0 = \ldots = a_{p-1} = 0$. Therefore these p rows are linearly independent, so the vectors $\{f^{\bullet i}\}_{i=0}^{p-1}$ are linearly independent.

For any $\lambda \in \mathbb{R}$, define $F_\lambda \in \{0,1\}^{[q]^n}$ by

$$F_\lambda(\mathbf{x}) = \begin{cases} 1 & F(\mathbf{x}) = \lambda \\ 0 & \text{otherwise} \end{cases},$$

and let F_λ have signature vector f_λ. The vector space $\langle f^{\bullet 0}, \dots f^{\bullet p-1}\rangle_+ \subset \langle f_\lambda \mid \lambda \in \mathbb{C}\rangle_+$, a space of dimension p, so, since $\{f^{\bullet i}\}_{i=0}^{p-1}$ are linearly independent, the reverse inclusion also holds: $\langle f^{\bullet 0}, \dots f^{\bullet p-1}\rangle_+ = \langle f_\lambda \mid \lambda \in \mathbb{C}\rangle_+$. Therefore each F_λ is quantum-gadget realizable, as each $F^{\bullet i}$ is gadget-realizable, so

$$\{M(\mathbf{Q}) \mid \mathbf{Q} \in \mathfrak{Q}_{\mathcal{F}}(m,d)\} = \{M(\mathbf{Q}) \mid \mathbf{Q} \in \mathfrak{Q}_{\{F_\lambda \mid F \in \mathcal{F}, \lambda \in \mathbb{C}\}}(m,d)\}. \tag{6}$$

By the $\subset$ inclusion of Theorem 16, each $f^{\bullet i} \in \langle E^{1,0}, E^{1,2}, S^{2,2}, \{f \mid F \in \mathcal{F}\}\rangle_{\circ,\otimes,\dagger}$ as well, so, similarly,

$$\begin{aligned} C_{\mathrm{Aut}(\mathcal{F})} &= \langle E^{1,0}, E^{1,2}, S^{2,2}, \{f \mid F \in \mathcal{F}\}\rangle_{\circ,\otimes,\dagger} \\ &= \langle E^{1,0}, E^{1,2}, S^{2,2}, \{f_\lambda \mid F \in \mathcal{F}, \lambda \in \mathbb{C}\}\rangle_{\circ,\otimes,\dagger} = C_{\mathrm{Aut}(\{F_\lambda \mid F \in \mathcal{F}, \lambda \in \mathbb{C}\})} \end{aligned} \tag{7}$$

(with the first and third equalities using Theorem 20). Now, applying (5) to the $\mathbb{R}$-valued set $\{F_\lambda \mid F \in \mathcal{F}, \lambda \in \mathbb{C}\}$, along with (6) and (7), gives

$$\begin{aligned} C_{\mathrm{Aut}(\mathcal{F})} = C_{\mathrm{Aut}(\{F_\lambda \mid F \in \mathcal{F}, \lambda \in \mathbb{C}\})} &= \{M(\mathbf{Q}) \mid \mathbf{Q} \in \mathfrak{Q}_{\{F_\lambda \mid F \in \mathcal{F}, \lambda \in \mathbb{C}\}}(m,d)\} \\ &= \{M(\mathbf{Q}) \mid \mathbf{Q} \in \mathfrak{Q}_{\mathcal{F}}(m,d)\}. \end{aligned}$$

$\square$

Theorem 21 is an extension of [28, Theorem 8.5] and, in view of Proposition 17 and the equivalence between (m,d)-quantum $\{A_X\}$-gadgets and $(m+d)$-labeled quantum graphs, [26, Lemma 2.5] from graph homomorphism to #CSP. The next result similarly generalizes [26, Lemma 2.4]. It is also a version of Theorem 34 (proved by interpolation below) restricted to $\mathcal{F} = \mathcal{G}$.

Lemma 22. *Let $k > 0$ and $\varphi, \psi : [k] \to V(\mathcal{F})$. If $Z^\varphi(K) = Z^\psi(K)$ for every $K \in \mathcal{PLI}[\mathcal{F}; k]$, then $(\mathcal{F}, \varphi) \cong (\mathcal{F}, \psi)$.*

Proof. View K as a gadget $\mathbf{K} \in \mathfrak{G}_{\mathcal{F}}(k,0)$. Write $\varphi([k]) := (\varphi(0), \dots, \varphi(k-1)) \in V(\mathcal{F})^k$. Then, by assumption, for every $\mathbf{K} \in \mathfrak{G}_{\mathcal{F}}(k,0)$,

$$(M(\mathbf{K}))_{\varphi([k])} = Z^\varphi(K) = Z^\psi(K) = (M(\mathbf{K}))_{\psi([k])}.$$

Thus $(M(\mathbf{Q}))_{\varphi([k])} = (M(\mathbf{Q}))_{\psi([k])}$ for every $\mathbf{Q} \in \mathfrak{Q}_{\mathcal{F}}(k,0)$, so $v_{\varphi([k])} = v_{\psi([k])}$ for every $\mathbf{v} \in C_{\mathrm{Aut}(\mathcal{F})}(k,0)$ by Theorem 21. Then, by Proposition 17, there is a $\sigma \in \mathrm{Aut}(\mathcal{F})$ satisfying $\sigma(\varphi([k])) = \psi([k])$. In other words, $\sigma \circ \varphi = \psi$. $\square$

Definition 23 ($\oplus$)**.** Let $F \in \mathbb{F}^{V(F)^n}$, $G \in \mathbb{F}^{V(G)^n}$ be constraint functions of arity $n \geqslant 2$. Define the *direct sum* $F \oplus G \in \mathbb{F}^{(V(G) \sqcup V(F))^n}$ of F and G by, for $\mathbf{x} \in (V(F) \sqcup V(G))^n$,

$$(F \oplus G)(\mathbf{x}) = \begin{cases} F(\mathbf{x}) & \mathbf{x} \in V(F)^n \\ G(\mathbf{x}) & \mathbf{x} \in V(G)^n \\ 0 & \text{otherwise.} \end{cases}$$

For similar $\mathcal{F}$ and $\mathcal{G}$, define $\mathcal{F} \oplus \mathcal{G} = \{F \oplus G \mid \mathcal{F} \ni F \leftrightsquigarrow G \in \mathcal{G}\}$ on domain $V(\mathcal{F}) \sqcup V(\mathcal{G})$.

For $n = 2$, $F \oplus G$ is the adjacency matrix of the disjoint union of the $\mathbb{F}$-weighted graphs with adjacency matrices F and G.

Definition 24 ($\sim, \approx$, connected constraint function)**.** For a constraint function set $\mathcal{F}$, define an equivalence relation $\approx$ on $V(\mathcal{F})$ as the transitive closure of the relation $\sim$, where $y \sim z$ if there is an $F \in \mathcal{F}$ and a tuple $\mathbf{x} \in V(F)^{\text{arity}(F)}$ containing y and z such that $F(\mathbf{x}) \neq 0$. Say $\mathcal{F}$ is *connected* if $\approx$ has exactly one equivalence class, and is *disconnected* otherwise.

For $I \subset V(\mathcal{F})$, define $\mathcal{F}|_I := \{F|_I : F \in \mathcal{F}\}$, where $F|_I \in \mathbb{C}^{I^{\text{arity}(F)}}$ is the subtensor of F induced by I. If $I, J \subset V(\mathcal{F})$ are distinct equivalence classes of $\approx$ ('connected components') and $\sigma \in \text{Aut}(\mathcal{F})$ satisfies $\sigma(i) = j$ for some $i \in I$ and $j \in J$, it follows that σ is an isomorphism between $\mathcal{F}|_I$ and $\mathcal{F}|_J$. In particular, if $\mathcal{F}$ and $\mathcal{G}$ are connected, then $V(\mathcal{F})$ and $V(\mathcal{G})$ are the two equivalence classes of $V(\mathcal{F} \oplus \mathcal{G})$, so if there is a $\sigma \in \text{Aut}(\mathcal{F} \oplus \mathcal{G})$ mapping some $x \in V(\mathcal{F})$ to some $y \in V(\mathcal{G})$, then $\mathcal{F} \cong \mathcal{G}$. For $n = 2$ and symmetric F and G, the above statements are all equivalent to the corresponding well-known facts about graphs.

We now have all the tools needed to prove Theorem 8 for $\mathbb{F} = \mathbb{C}$.

Theorem 25. *let $\mathcal{F}$ and $\mathcal{G}$ be similar $\mathbb{C}$-valued constraint function sets. Then $\mathcal{F} \cong \mathcal{G}$ if and only if $\mathcal{F}$ and $\mathcal{G}$ are* #CSP*-indistinguishable.*

Proof. We only need the ($\Longleftarrow$) direction. Suppose $\mathcal{F}$ and $\mathcal{G}$ are #CSP-indistinguishable. Let 0_F and 0_G be new domain elements. For each $F \in \mathcal{F}$, $G \in \mathcal{G}$ of arity $n \geqslant 2$, define constraint functions F' and G' on $V(\mathcal{F}') := V(\mathcal{F}) \cup \{0_F\}$ and $V(\mathcal{G}') := V(\mathcal{G}) \cup \{0_G\}$, respectively, by

$$F'(\mathbf{x}) = \begin{cases} F(\mathbf{x}) & \mathbf{x} \in V(\mathcal{F})^n \\ 1 & \text{otherwise} \end{cases}, \qquad G'(\mathbf{x}) = \begin{cases} G(\mathbf{x}) & \mathbf{x} \in V(\mathcal{G})^n \\ 1 & \text{otherwise} \end{cases}$$

for $\mathbf{x} \in V(\mathcal{F}')^n$ and $\mathbf{x} \in V(\mathcal{G}')^n$, respectively. In other words, if any entry of $\mathbf{x}$ is 0_F, then $F'(\mathbf{x}) = 1$, and similarly for G'. For unary $F \in \mathcal{F}$, $G \in \mathcal{G}$, define *binary* F' and G' by

$$F'(x, y) = \begin{cases} F(x) & x = y \in V(\mathcal{F}) \\ 1 & x = 0_F \text{ or } y = 0_F \\ 0 & \text{otherwise} \end{cases}, \qquad G'(x, y) = \begin{cases} G(x) & x = y \in V(\mathcal{G}) \\ 1 & x = 0_G \text{ or } y = 0_G \\ 0 & \text{otherwise} \end{cases}$$

for $x, y \in V(\mathcal{F}')$ and $x, y \in V(\mathcal{G}')$, respectively. The arity increase is necessary because connectivity only makes sense for constraint functions with arity at least two. Now let $\mathcal{F}' = \{F' \mid F \in \mathcal{F}\}$ and $\mathcal{G}' = \{G' \mid G \in \mathcal{G}\}$.

Let $K = (V, C) \in \mathcal{PLI}[\mathcal{F}' \oplus \mathcal{G}'; 1]$ be a 1-labeled #CSP($\mathcal{F}' \oplus \mathcal{G}'$) instance, with labeled variable $v_0 \in V$. We will show that

$$Z^{0 \mapsto 0_F}(K) = Z^{0 \mapsto 0_G}(K). \tag{8}$$

If K is not connected (i.e. the underlying graph of the Holant($\mathcal{F} \mid \mathcal{EQ}$) signature grid corresponding to K is not connected), then the components of K that do not contain v_0 contribute the same value to the partition regardless of the assignment to v_0. Hence, to establish (8), we may assume K is connected. Therefore, if $\phi : V \to V(\mathcal{F}' \oplus \mathcal{G}')$ satisfies $\phi(v_0) = 0_F$, then, since each $F' \oplus G'$ evaluates to 0 unless all its inputs are in $V(\mathcal{F}')$ or all its inputs are in $V(\mathcal{G}')$, we must have $\phi(V) \subset V(\mathcal{F}')$ for any ϕ contributing a nonzero value to $Z^{0 \mapsto 0_F}(K)$.

Any ϕ with $\phi(v_0) = 0_F$ maps some $S \subset V$ to 0_F, with $v_0 \in S$. For a fixed $S \subset V$, the remaining variables $V \setminus S$ take all values in $V(\mathcal{F}') \setminus \{0_F\} = V(\mathcal{F})$ as ϕ ranges over $\{\phi \mid \phi^{-1}(0_F) = S\}$. Additionally, any constraint containing a variable in S always evaluates to 1, regardless of the assignments to the other variables. Construct a #CSP($\mathcal{F}$) instance $K^{\mathcal{F}}_{V \setminus S}$ from K as follows. First eliminate all variables in S and all constraints containing any variable in S. Then, for each constraint applying $F' \oplus G'$, if F and G have arity > 1, replace $F' \oplus G'$ with F. If F and G are unary, then merge the two variables to which the binary $F' \oplus G'$ is applied and replace the constraint with a constraint applying F to the merged variable. Assuming all inputs to $F' \oplus G'$ are in $V(\mathcal{F})$, this variable merging procedure does not change the value of the partition function, since by construction $F' \oplus G'$ acts as the function $(x, y) \mapsto \delta_{xy} F_x$. Now the total contribution to $Z^{0 \mapsto 0_F}(K)$ of the assignments ϕ satisfying $\phi^{-1}(0_F) = S$ is $Z(K^{\mathcal{F}}_{V \setminus S})$. Thus

$$Z^{0 \mapsto 0_F}(K) = \sum_{S \subset V, S \ni v_0} Z(K^{\mathcal{F}}_{V \setminus S}).$$

A similar expression holds for $Z^{0 \mapsto 0_G}(K)$, with the #CSP($\mathcal{G}$) instance $K^{\mathcal{G}}_{V \setminus S} = (K^{\mathcal{F}}_{V \setminus S})_{\mathcal{F} \to \mathcal{G}}$ in place of $K^{\mathcal{F}}_{V \setminus S}$. So, by assumption,

$$Z^{0 \mapsto 0_F}(K) = \sum_{S \subset V, S \ni v_0} Z(K^{\mathcal{F}}_{V \setminus S}) = \sum_{S \subset V, S \ni v_0} Z(K^{\mathcal{G}}_{V \setminus S}) = Z^{0 \mapsto 0_G}(K),$$

proving (8). Now by Lemma 22 with $k = 1$, there is a $\sigma \in \operatorname{Aut}(\mathcal{F}' \oplus \mathcal{G}')$ satisfying $\sigma(0_F) = 0_G$. By construction, 0_F and 0_G satisfy $0_F \sim x$ for every $x \in V(\mathcal{F}')$ and $0_G \sim y$ for every $y \in V(\mathcal{G}')$, so $\mathcal{F}'$ and $\mathcal{G}'$ are connected. Therefore $\sigma|_{V(\mathcal{F}')}$ is an isomorphism between $\mathcal{F}'$ and $\mathcal{G}'$. But $\sigma(0_F) = 0_G$, so $\sigma|_{V(\mathcal{F})}$ is an isomorphism between $\mathcal{F}$ and $\mathcal{G}$ (if F and G are unary, then $\sigma|_{V(\mathcal{F})}$ is really an isomorphism between the functions $(x, y) \mapsto \delta_{xy} F_y$ and $(x, y) \mapsto \delta_{xy} G_y$, but this implies an isomorphism between F and G, since unary functions are isomorphic if and only if they have the same multiset of entries). $\square$

The proof of Theorem 25 is a 'classical' version of Cai and Young's proof of [13, Lemma 14], and a generalization of Lovász's proof of [26, Corollary 2.6], which is essentially Theorem 8 restricted to real-weighted graph homomorphism. Both proofs use the idea of adding a universal vertex to connect the graph/constraint function, since for weighted such objects we cannot take the complement to assume connectedness.

4 The Interpolation Proof

4.1 Preliminaries

Here, we introduce some definitions specific to the interpolation proof. First, define a domain-weighted #CSP problem.

Definition 26 (#CSP$(\boldsymbol{\mathcal{F}}, \boldsymbol{\alpha})$, $\boldsymbol{Z_{\alpha}^{\psi}}$)**.** The problem #CSP$(\mathcal{F}, \alpha)$ is parameterized by a set $\mathcal{F}$ of constraint functions and a vector $\alpha \in (\mathbb{F} \setminus \{0\})^{V(\mathcal{F})}$ of *domain weights*. The partition function Z_{α}^{ψ}, defined on #CSP$(\mathcal{F})$ instances $K = (V, C)$, is

$$Z_{\alpha}^{\psi}(K) = \sum_{\phi: V \to V(\mathcal{F}) \text{ extends } \psi} \frac{\alpha_\phi}{\alpha_\psi} \prod_{(F, v_1, \ldots, v_{n_F}) \in C} F(\phi(v_1), \ldots, \phi(v_{n_F})),$$

where

$$\alpha_\phi = \prod_{v \in V} \alpha_{\phi(v)} \text{ and } \alpha_\psi = \prod_{i \in [k]} \alpha_{\psi(i)}.$$

In particular, $Z_{\mathbf{1}}^{\psi} = Z^{\psi}$, where $\mathbf{1}$ is the all-ones vector. One can model domain weights in the ordinary #CSP setting by applying a unary constraint function to each variable. However, explicit domain weights will prove useful for removing twin domain elements in Corollary 35, so we consider them separately.

Call $(\mathcal{F}, \alpha, \varphi)$ and $(\mathcal{G}, \beta, \psi)$ (simple)-#CSP-indistinguishable if $Z_{\alpha}^{\varphi}(K) = Z_{\beta}^{\psi}(K_{\mathcal{F} \to \mathcal{G}})$ for every $K \in \mathcal{PLI}[\mathcal{F}; k]$ (resp. $\mathcal{PLI}^{\text{simp}}[\mathcal{F}; k]$), and say σ is an isomorphism of $(\mathcal{F}, \alpha, \varphi)$ and $(\mathcal{G}, \beta, \psi)$ if σ is an isomorphism of $(\mathcal{F}, \varphi)$ and $(\mathcal{G}, \psi)$ and $\alpha_i = \beta_{\sigma(i)}$ for all $i \in V(\mathcal{F})$.

For $\mathcal{F} = \{F_j \mid j \in T\}$ indexed by a possibly infinite set T, define the following set, which represents all 'configurations' of the remaining arguments of an application of a function in $\mathcal{F}$ when given a single distinguished argument at position r:

$$\mathcal{J}(\mathcal{F}) := \{(j, \mathbf{x}, r) \mid j \in T, \mathbf{x} \in V(\mathcal{F})^{n_j - 1}, r \in [n_j]\}, \tag{9}$$

where n_j is the arity of $F_j \in \mathcal{F}$. If $n_j = 1$ (F_j is unary), then say $V(\mathcal{F})^{n_j - 1} = V(\mathcal{F})^0 = \{()\}$ (the set containing the empty tuple). For a length-n tuple $\mathbf{x}$, index $r \in [n+1]$ and any y, define $\mathbf{x}^{r \hookleftarrow y}$ as the length-$n+1$ tuple $(x_0, \ldots, x_{r-1}, y, x_r, \ldots, x_{n-1})$ created by inserting y at position r. Domain elements $i, i' \in V(\mathcal{F})$ are *twins* if

$$F_j\left(\mathbf{x}^{r \hookleftarrow i}\right) = F_j\left(\mathbf{x}^{r \hookleftarrow i'}\right) \text{ for every } (j, \mathbf{x}, r) \in \mathcal{J}(\mathcal{F}).$$

If $n_j = 1$ and $\mathbf{x} = ()$, then $F_j\left(\mathbf{x}^{r \hookleftarrow i}\right) = F_j(i)$. If every $F \in \mathcal{F}$ is symmetric, meaning F is invariant under permutations of the order of its inputs, then say $\mathcal{F}$ is symmetric, and

$i, i' \in V(\mathcal{F})$ are twins if $F_j(i, \mathbf{x}) = F_j(i', \mathbf{x})$ for every $j \in T$ and $\mathbf{x} \in V(\mathcal{F})^{n_j - 1}$, where we abbreviate $F_j(i, \mathbf{x}) = F_j\big(\mathbf{x}^{0 \hookleftarrow i}\big)$. $\mathcal{F}$ is *twin-free* if no two domain elements are twins. Equivalently, $\mathcal{F}$ is twin-free iff the tuples

$$\big(F_j\big(\mathbf{x}^{r \hookleftarrow i}\big)\big)_{(j,\mathbf{x},r) \in \mathcal{J}(\mathcal{F})}$$

are pairwise distinct for $i \in V(\mathcal{F})$. If $\mathcal{F}$ is symmetric, then $\mathcal{F}$ is twin free if and only if the tuples $(F_j(i, \mathbf{x}))_{j \in T, \mathbf{x} \in V(\mathcal{F})^{n_j - 1}}$ are pairwise distinct for $i \in V(\mathcal{F})$.

4.1.1 Vandermonde Interpolation

Next, we introduce the iterated Vandermonde interpolation lemma of Cai and Govorov [12], which follows from iterated applications of Proposition 1.

Lemma 27 ([12, Corollary 4.2])**.** *Let I and J be finite index sets, and a_i, $b_{i,j} \in \mathbb{F}$ for all $i \in I$, $j \in J$. Further, let $I = \bigsqcup_{\ell \in [s]} I_\ell$ be the partition of I into equivalence classes defined by relation $\sim$, where $i \sim i'$ iff $b_{i,j} = b_{i',j}$ for all $j \in J$. If*

$$\sum_{i \in I} a_i \prod_{j \in J} b_{i,j}^{p_j} = 0$$

for all choices of $(p_j)_{j \in J}$ where each $0 \leqslant p_j < |I|$, then $\sum_{i \in I_\ell} a_i = 0$ for every $\ell \in [s]$.

In this work, I (and J) will often be the set of all m-tuples whose entries range over a fixed finite set. In this case, we have the following corollary.

Corollary 28. *Let I and J be finite index sets and $m \geqslant 1$. Let $a_{\mathbf{i}} \in \mathbb{F}$ for $\mathbf{i} \in I^m$ and $b_{i,j} \in \mathbb{F}$ for $i \in I, j \in J$. Define $\sim$ as in Lemma 27. Let $I^m = \bigsqcup_{k \in [s_m]} I_k^{(m)}$ be a partition of I^m into equivalence classes defined by relation $\sim_m$, where $\mathbf{i} \sim_m \mathbf{i}'$ if $i_h \sim i'_h$ for all $h \in [m]$. If*

$$\sum_{\mathbf{i} \in I^m} a_{\mathbf{i}} \prod_{j \in J, h \in [m]} b_{i_h,j}^{p_{h,j}} = 0 \tag{10}$$

for every choice of $(p_{h,j})_{j \in J, h \in [m]}$, where each $0 \leqslant p_{h,j} < |I|$, then, for every $k \in [s_m]$,

$$\sum_{\mathbf{i} \in I_k^{(m)}} a_{\mathbf{i}} = 0.$$

Proof. Apply induction on m. The case $m = 1$ is exactly Lemma 27. Otherwise, assume Corollary 28 holds for $m - 1$ and any choice of $a_{(i_0,\ldots,i_{m-2})}$ for each $(i_0, \ldots, i_{m-2}) \in I^{m-1}$. Separating the sum in (10) over i_{m-1} gives

$$\sum_{i_{m-1} \in I} \left(\sum_{(i_0,\ldots,i_{m-2}) \in I^{m-1}} a_{\mathbf{i}} \prod_{j \in J, h \in [m-1]} b_{i_h,j}^{p_{h,j}} \right) \left(\prod_{j \in J} b_{i_{m-1},j}^{p_{m-1,j}} \right) = 0. \tag{11}$$

Now apply Lemma 27 with $i := i_{m-1}$ and

$$a_{i_{m-1}} := \sum_{(i_0,\dots,i_{m-2})\in I^{m-1}} a_{\mathbf{i}} \prod_{j\in J, h\in[m-1]} b_{i_h,j}^{p_{h,j}} \quad \text{and} \quad p_j := p_{m-1,j}.$$

For every $\ell \in [s]$ (with s and $(I_\ell)_{\ell\in[s]}$ from Lemma 27), we obtain

$$0 = \sum_{i_{m-1}\in I_\ell} a_{i_{m-1}} = \sum_{i_{m-1}\in I_\ell} \left(\sum_{(i_0,\dots,i_{m-2})\in I^{m-1}} a_{\mathbf{i}} \prod_{j\in J, h\in[m-1]} b_{i_h,j}^{p_{h,j}} \right)$$
$$= \sum_{(i_0,\dots,i_{m-2})\in I^{m-1}} \left(\sum_{i_{m-1}\in I_\ell} a_{\mathbf{i}} \right) \prod_{j\in J, h\in[m-1]} b_{i_h,j}^{p_{h,j}}.$$

Now, inductively applying Corollary 28 with, for each $(i_0,\dots,i_{m-2}) \in I^{m-1}$,

$$a_{(i_0,\dots,i_{m-2})} := \sum_{i_{m-1}\in I_\ell} a_{\mathbf{i}},$$

we conclude that, for every $k' \in [s_{m-1}]$,

$$\sum_{(i_0,\dots,i_{m-2})\in I_{k'}^{(m-1)}} \sum_{i_{m-1}\in I_\ell} a_{\mathbf{i}} = 0. \tag{12}$$

By definition, $(i_0,\dots,i_{m-2}) \sim_{m-1} (i'_0,\dots,i'_{m-2}) \wedge i_{m-1} \sim i'_{m-1} \iff \mathbf{i} \sim_m \mathbf{i}'$. Hence, for fixed k' and ℓ, the double sum in (12) is a sum over a single equivalence class $I_k^{(m)}$, and since (12) holds for every choice of $k' \in [s_{m-1}]$ and $\ell \in [s]$, we obtain the desired $\sum_{\mathbf{i}\in I_k^{(m)}} a_{\mathbf{i}} = 0$ for every $k \in [s_m]$. ☐

4.2 The Unary Case

First, we must separately address the case where $\mathcal{F}$ and $\mathcal{G}$ contain only unary constraint functions, where Lemma 32 below does not apply. The proof uses simple versions of the arguments we will apply throughout this section.

Lemma 29. *Let $(\mathcal{F},\alpha)$ and $(\mathcal{G},\beta)$ be finite similar domain-weighted sets of unary constraint functions with $|V(\mathcal{F})| \geqslant |V(\mathcal{G})|$. Assume $\mathcal{F}$ is twin-free. Let $k \geqslant 0$ and $\varphi : [k] \to V(\mathcal{F})$ and $\psi : [k] \to V(\mathcal{G})$. If $(\mathcal{F},\alpha,\varphi)$ and $(\mathcal{G},\beta,\psi)$ are simple-#CSP-indistinguishable, then $|V(\mathcal{F})| = |V(\mathcal{G})|$ and $(\mathcal{F},\alpha,\varphi) \cong (\mathcal{G},\beta,\psi)$.*

Proof. Write $\mathcal{F} = \{F_i \mid i \in [t]\}$ and $\mathcal{G} = \{G_i \mid i \in [t]\}$. For $\mathbf{p} \in [|V(\mathcal{F}) \sqcup V(\mathcal{G})|]^t$, let $K^{\mathbf{p}} \in \mathcal{PLI}^{\text{simp}}[\mathcal{F};k]$ be the instance with an unlabeled variable v, k unused labeled variables, and p_j copies of the constraint (F_j, v), for $j \in [t]$. Then $Z_\alpha^\varphi(K^{\mathbf{p}}) = Z_\beta^\psi(K^{\mathbf{p}}_{\mathcal{F}\to\mathcal{G}})$ is equivalent to

$$\sum_{i\in V(\mathcal{F})} \alpha_i \prod_{j\in[t]} F_j(i)^{p_j} + \sum_{i\in V(\mathcal{G})} (-\beta_i) \prod_{j\in[t]} G_j(i)^{p_j} = 0. \tag{13}$$

Considering (13) for every $\mathbf{p} \in [|V(\mathcal{F}) \sqcup V(\mathcal{G})|]^t$, we may apply Lemma 27 with $I := V(\mathcal{F}) \sqcup V(\mathcal{G})$, $J := [t]$, $a_i := \alpha_i$ or β_i, and $b_{i,j} := F_j(i)$ or $G_j(i)$ for $i \in V(\mathcal{F})$ or $i \in V(\mathcal{G})$, respectively. As $\mathcal{F}$ is twin-free, the tuples $(b_{i,j})_{j\in[t]} = (F_j(i))_{j\in[t]}$ are distinct for distinct $i \in V(\mathcal{F})$. Therefore no equivalence class I_ℓ from Lemma 27 contains more than one element of $V(\mathcal{F})$. However, every $\alpha_i \neq 0$ by definition, so no equivalence class consists of only a single element of $V(\mathcal{F})$. Thus there is a function $\sigma : V(\mathcal{F}) \to V(\mathcal{G})$ such that $i \sim \sigma(i)$ – or equivalently $\forall j \in [t] : F_j(i) = b_{i,j} = b_{\sigma(i),j} = G_j(\sigma(i))$ – for every $i \in V(\mathcal{F})$. Furthermore, since no two elements of $V(\mathcal{F})$ are in the same equivalence class, σ is injective, hence bijective, as $|V(\mathcal{F})| \geqslant |V(\mathcal{G})|$. Therefore $|V(\mathcal{F})| = |V(\mathcal{G})|$, and Lemma 27 concludes that $\alpha_i - \beta_{\sigma(i)} = 0$ for every $i \in V(\mathcal{F})$, so σ is an isomorphism of $(\mathcal{F}, \alpha)$ and $(\mathcal{G}, \beta)$.

Now, for every $c \in [k]$ and $F \in \mathcal{F}$, let $K^{F,c} \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; k]$ be an instance with k labeled variables, no unlabeled variables, and a single constrant applying F to the variable labeled c. Then

$$F(\varphi(c)) = Z^\varphi_\alpha(K^{F,c}) = Z^\psi_\beta(K^{F,c}_{\mathcal{F}\to\mathcal{G}}) = G(\psi(c)) = F(\sigma^{-1}(\psi(c))),$$

where $G \leftrightsquigarrow F$. By twin-freeness of $\mathcal{F}$, we conclude that $\varphi(c) = \sigma^{-1}(\psi(c))$. Therefore $\psi = \sigma \circ \varphi$. $\square$

4.3 The Symmetric Ternary Case

For clarity of exposition, we first prove the key lemma for the special case in which all constraint functions are symmetric and ternary.

Proposition 30. *Let $\mathcal{F} = \{F_j \mid j \in [t]\}$ and $\mathcal{G} = \{G_j \mid j \in [t]\}$ be finite similar constraint function sets with $|V(\mathcal{F})| \geqslant |V(\mathcal{G})|$ such that every $F \in \mathcal{F}$ and $G \in \mathcal{G}$ are symmetric and have arity 3, and assume $\mathcal{F}$ is twin-free. Let α, β be the domain weights associated with $\mathcal{F}$ and $\mathcal{G}$, respectively.*

Let $\theta : [2k] \to V(\mathcal{F})$ and $\psi : [2k] \to V(\mathcal{G})$ for $k \geqslant 0$, and for every $x, y \in V(\mathcal{F})$, let

$$I_{xy} = \{a \in [k] \mid (\theta(a), \theta(a+k)) = (x, y)\} \subset [k]$$

Assume θ is well-balanced *– that is, for every $x, y \in V(\mathcal{F})$, $|I_{xy}| \geqslant 2|V(\mathcal{F})|^3$. If $Z^\theta_\alpha(K) = Z^\psi_\beta(K_{\mathcal{F}\to\mathcal{G}})$ for every $K \in \mathcal{PLI}^{simp}[\mathcal{F}; 2k]$, then $|V(\mathcal{F})| = |V(\mathcal{G})|$ and $(\mathcal{F}, \alpha, \theta) \cong (\mathcal{G}, \beta, \psi)$.*

Proof. By the pigeonhole principle, since $|I_{xy}| \geqslant 2|V(\mathcal{F})|^3 \geqslant 2|V(\mathcal{F})| \cdot |V(\mathcal{G})|^2$ for every $x, y \in V(\mathcal{F})$, there exists a function $s : V(\mathcal{F})^2 \to V(\mathcal{G})^2$ such that for every $x, y \in V(\mathcal{F})$, the set

$$J_{xy} := I_{xy} \cap \{a \in [k] \mid (\psi(a), \psi(a+k)) = s(x, y)\}$$

satisfies $|J_{xy}| \geqslant 2|V(\mathcal{F})|$. Consider the variable set

$$V_1 = \{v, u_0, \ldots, u_{2k-1}\},$$

where each u_ℓ is labeled ℓ. For each choice of $\mathbf{p} = (p_{xyj})_{x,y\in V(\mathcal{F}),j\in[t]} \in [2|V(\mathcal{F})|]^{V(\mathcal{F})^2\times[t]}$, construct a $2k$-labeled #CSP($\mathcal{F}$) instance $K^{\mathbf{p}} \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; 2k]$ as follows. For each $x, y \in V(\mathcal{F})$ and $j \in [t]$, choose an arbitrary $P_{xyj} \subset J_{xy}$ with $|P_{xyj}| = p_{xyj}$, and define

$$C^{\mathbf{p}}(v) := \bigcup_{x,y\in V(\mathcal{F})} \bigcup_{j\in[t]} \bigcup_{a\in P_{xyj}} (F_j, v, u_a, u_{a+k}). \tag{14}$$

Then define $K^{\mathbf{p}} := (V_1, C^{\mathbf{p}}(v))$. If $a \in P_{xyj} \subset J_{xy}$, then by definition $(\theta(a), \theta(a+k)) = (x, y)$ and $(\psi(a), \psi(a+k)) = s(x, y)$. Hence the variables (u_a, u_{a+k}) take values (x, y) and $s(x, y)$ under θ and ψ, respectively, independent of the choice of a in P_{xyj}. Therefore $Z^\theta_\alpha(K^{\mathbf{p}}) = Z^\psi_\beta(K^{\mathbf{p}}_{\mathcal{F}\to\mathcal{G}})$ is equivalent to

$$\sum_{i\in V(\mathcal{F})} \alpha_i \prod_{x,y\in V(\mathcal{F}),j\in[t]} F_j(i, x, y)^{p_{xyj}} + \sum_{i\in V(\mathcal{G})} (-\beta_i) \prod_{x,y\in V(\mathcal{G}),j\in[t]} G_j(i, s(x, y))^{p_{xyj}} = 0, \tag{15}$$

where we write $G_j(i, s(x, y))$ to mean $G_j(i, s(x, y)_0, s(x, y)_1)$. The sums over i correspond to the choice of assignment for the only free variable v in $K^{\mathbf{p}}$ and $K^{\mathbf{p}}_{\mathcal{F}\to\mathcal{G}}$, respectively. Overall, the LHS of (15) is a sum over $V(\mathcal{F}) \sqcup V(\mathcal{G})$, with $|V(\mathcal{F}) \sqcup V(\mathcal{G})| = |V(\mathcal{F})| + |V(\mathcal{G})| \leqslant 2|V(\mathcal{F})|$. By constructing $K^{\mathbf{p}}$ and considering (15) for every $\mathbf{p} \in [2|V(\mathcal{F})|]^{V(\mathcal{F})^2\times[t]}$, we may apply Lemma 27 with

$$\begin{gathered} I := V(\mathcal{F}) \sqcup V(\mathcal{G}),\ J := V(\mathcal{F})^2 \times [t], \\ a_i := \begin{cases} \alpha_i & i \in V(\mathcal{F}) \\ -\beta_i & i \in V(\mathcal{G}) \end{cases},\ b_{i,xyj} := \begin{cases} F_j(i, x, y) & i \in V(\mathcal{F}) \\ G_j(i, s(x, y)) & i \in V(\mathcal{G}) \end{cases}. \end{gathered}$$

Since $\mathcal{F}$ is twin-free, the tuples $(F_j(i, x, y))_{x,y\in V(\mathcal{F}),j\in[t]}$ are pairwise distinct for $i \in V(\mathcal{F})$. Hence no equivalence class contains more than one element of $V(\mathcal{F})$. However, every $\alpha_i \neq 0$, so no equivalence class consists of only a single element of $V(\mathcal{F})$. Thus there is a function $\sigma : V(\mathcal{F}) \to V(\mathcal{G})$ such that $i \sim \sigma(i)$ for every $i \in V(\mathcal{F})$ – that is,

$$(F_j(i, x, y))_{x,y\in V(\mathcal{F}),j\in[t]} = (G_j(\sigma(i), s(x, y)))_{x,y\in V(\mathcal{F}),j\in[t]} \text{ for every } i \in V(\mathcal{F}). \tag{16}$$

Since no two elements of $V(\mathcal{F})$ are in the same equivalence class, σ is injective, hence bijective, as $|V(\mathcal{F})| \geqslant |V(\mathcal{G})|$. Therefore $|V(\mathcal{F})| = |V(\mathcal{G})|$, and Lemma 27 gives

$$\alpha_i = \beta_{\sigma(i)} \text{ for } i \in V(\mathcal{F}). \tag{17}$$

Next, we improve σ to an isomorphism between $(\mathcal{F}, \alpha)$ and $(\mathcal{G}, \beta)$. Define another family of #CSP($\mathcal{F}$) instances as follows. First, construct a $2k$-labeled variable set

$$V_2 := V_1 \cup \{v', v''\}$$

with two new variables v', v''. Fix $\mathcal{F} \ni F \leftrightsquigarrow G \in \mathcal{G}$. For $\mathbf{p}, \mathbf{p}', \mathbf{p}'' \in [|V(\mathcal{F})|]^{V(\mathcal{F})^2\times[t]}$, define (recall (14))

$$C^{F,\mathbf{p},\mathbf{p}',\mathbf{p}''} = \{(F, v, v', v'')\} \cup C^{\mathbf{p}}(v) \cup C^{\mathbf{p}'}(v') \cup C^{\mathbf{p}''}(v''),$$

a set of constraints on V_2, and define $K^{F,\mathbf{p},\mathbf{p}',\mathbf{p}''} = (V_2, C^{F,\mathbf{p},\mathbf{p}',\mathbf{p}''}) \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; 2k]$. Now $Z^\theta_\alpha(K^{F,\mathbf{p},\mathbf{p}',\mathbf{p}''}) = Z^\psi_\beta(K^{F,\mathbf{p},\mathbf{p}',\mathbf{p}''}_{\mathcal{F}\to\mathcal{G}})$ is equivalent to

$$\begin{aligned} 0 = &\sum_{i,i',i''\in V(\mathcal{F})} \alpha_i\alpha_{i'}\alpha_{i''} F(i,i',i'') \\ &\qquad\cdot \prod_{x,y\in V(\mathcal{F}),j\in[t]} F_j(i,x,y)^{p_{xyj}} F_j(i',x,y)^{p'_{xyj}} F_j(i'',x,y)^{p''_{xyj}} \\ &+ \sum_{i,i',i''\in V(\mathcal{G})} -\beta_i\beta_{i'}\beta_{i''} G(i,i',i'') \\ &\qquad\cdot \prod_{x,y\in V(\mathcal{G}),j\in[t]} G_j(i,s(x,y))^{p_{xyj}} G_j(i',s(x,y))^{p'_{xyj}} G_j(i'',s(x,y))^{p''_{xyj}} \end{aligned}$$

(where $F \leftrightsquigarrow G \in \mathcal{G}$). Applying (17) and (16) then gives

$$\begin{aligned} 0 = &\sum_{i,i',i''\in V(\mathcal{F})} \alpha_i\alpha_{i'}\alpha_{i''} \big(F(i,i',i'') - G(\sigma(i),\sigma(i'),\sigma(i''))\big) \\ &\qquad\cdot \prod_{x,y,j} F_j(i,x,y)^{p_{xyj}} F_j(i',x,y)^{p'_{xyj}} F_j(i'',x,y)^{p''_{xyj}}. \end{aligned} \tag{18}$$

Constructing $K^{F,\mathbf{p},\mathbf{p}',\mathbf{p}''}$ and considering (18) for all choices of $\mathbf{p},\mathbf{p}',\mathbf{p}'' \in [|V(\mathcal{F})|]^{V(\mathcal{F})^2\times[t]}$, we may apply Corollary 28 with

$$\begin{aligned} &m := 3,\ J = V(\mathcal{F})^2\times[t],\ a_{i,i',i''} := \alpha_i\alpha_{i'}\alpha_{i''}\big(F(i,i',i'') - G(\sigma(i),\sigma(i'),\sigma(i''))\big), \\ &b_{i_h,xyj} := F_j(i_h,x,y),\ p_{1,xyj} := p_{xyj},\ p_{2,xyj} := p'_{xyj},\ p_{3,xyj} := p''_{xyj}. \end{aligned}$$

Again, by twin-freeness, the tuples $(F_j(i,x,y))_{xyj}$ are pairwise distinct for $i \in V(\mathcal{F})$, so, for distinct (i,i',i''), the tuples

$$(F_j(i,x,y), F_j(i',x,y), F_j(i'',x,y))_{xyj}$$

are distinct. Now Corollary 28 gives $\alpha_i\alpha_{i'}\alpha_{i''}(F(i,i',i'') - G(\sigma(i),\sigma(i'),\sigma(i''))) = 0$ for all i,i',i''. Since each $\alpha_i \neq 0$ and our choice of F was arbitrary, this implies

$$F(i,i',i'') = G(\sigma(i),\sigma(i'),\sigma(i'')) \text{ for every } i,i',i'' \in V(\mathcal{F}) \text{ and every pair } F \leftrightsquigarrow G. \tag{19}$$

Combined with (17), (19) implies that σ is a isomorphism between $(\mathcal{F},\alpha)$ and $(\mathcal{G},\beta)$.

To conclude that $(\mathcal{F},\alpha,\theta) \cong (\mathcal{G},\beta,\psi)$, it remains to show that $\psi = \sigma\circ\theta$. Again let $\mathcal{F} \ni F \leftrightsquigarrow G \in \mathcal{G}$. Define a third family of #CSP($\mathcal{F}$) instances. Define a $2k$-labeled variable set

$$V_3 := V_1 \cup \{v'\} = V_2 \setminus \{v''\}.$$

Fix $c \in [2k]$ and, for $\mathbf{p},\mathbf{p}' \in [|V(\mathcal{F})|]^{V(\mathcal{F})^2\times[t]}$, define the following set of constraints on V_3:

$$C^{F,\mathbf{p},\mathbf{p}'} := \{(F,u_c,v,v')\} \cup C^{\mathbf{p}}(v) \cup C^{\mathbf{p}'}(v')$$

and let $K^{F,\mathbf{p},\mathbf{p}'} = (V_3, C^{F,\mathbf{p},\mathbf{p}'}) \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; 2k]$. Now $Z^{\theta}_{\alpha}(K^{F,\mathbf{p},\mathbf{p}'}) = Z^{\psi}_{\beta}(K^{F,\mathbf{p},\mathbf{p}'}_{\mathcal{F}\to\mathcal{G}})$ is equivalent to

$$\begin{aligned} 0 = &\sum_{i,i' \in V(\mathcal{F})} \alpha_i \alpha_{i'} F(\theta(c), i, i') \prod_{x,y,j} F_j(i,x,y)^{p_{xyj}} F_j(i',x,y)^{p'_{xyj}} \\ &+ \sum_{i,i' \in V(\mathcal{G})} -\beta_i \beta_{i'} G(\psi(c), i, i') \prod_{x,y,j} G_j(i, s(x,y))^{p_{xyj}} G_j(i', s(x,y))^{p'_{xyj}}. \end{aligned}$$

Applying (17) and (16) then gives

$$\sum_{i,i' \in V(\mathcal{F})} \alpha_i \alpha_{i'} \big(F(\theta(c), i, i') - G(\psi(c), \sigma(i), \sigma(i'))\big) \prod_{x,y,j} F_j(i,x,y)^{p_{xyj}} F_j(i',x,y)^{p'_{xyj}} = 0.$$

As above, the tuples $(F_j(i,x,y), F_j(i',x,y))_{xyj}$ are distinct for distinct (i,i'), so by a similar application of Corollary 28 with $m := 2$, we have $F(\theta(c), i, i') = G(\psi(c), \sigma(i), \sigma(i'))$ for all $i, i' \in V(\mathcal{F})$. This holds for any pair $F \leftrightsquigarrow G$, so, by (19),

$$F_j(\theta(c), i, i') = G_j(\psi(c), \sigma(i), \sigma(i')) = F_j(\sigma^{-1}(\psi(c)), i, i')$$

for all $i, i' \in V(\mathcal{F})$ and $j \in [t]$. Since $\mathcal{F}$ is twin-free, we have $\theta(c) = \sigma^{-1}(\psi(c))$, hence $\sigma(\theta(c)) = \psi(c)$. We chose $c \in [2k]$ arbitrarily, so $\psi = \sigma \circ \theta$. $\square$

4.4 The General Case

We now extend Proposition 30 to general finite sets of arbitrary arity, non-necessarily-symmetric constraint functions, containing at least one non-unary constraint function.

Definition 31. Let $(\mathcal{F}, \alpha)$ be a domain-weighted constraint function set. Say $\theta : [k] \to V(\mathcal{F})$ is an *isomorphism pinning* for $(\mathcal{F}, \alpha)$ if, for any similar domain-weighted constraint function set $(\mathcal{G}, \beta)$ with $|V(\mathcal{G})| \leqslant |V(\mathcal{F})|$ and any $\psi : [k] \to V(\mathcal{G})$, if $(\mathcal{F}, \alpha, \theta)$ and $(\mathcal{G}, \beta, \psi)$ are simple-#CSP-indistinguishable, then $|V(\mathcal{F})| = |V(\mathcal{G})|$ and $(\mathcal{F}, \alpha, \theta) \cong (\mathcal{G}, \beta, \psi)$.

Lemma 32. *Let $\mathcal{F} = \{F_j \mid j \in [t]\}$ be twin-free, with domain weights α. Let $n = \max_{j\in[t]} n_j$ be the maximum arity among all functions in $\mathcal{F}$, and assume $n \geqslant 2$. Suppose $\theta : [(n-1)k] \to V(\mathcal{F})$, and for every $\mathbf{x} \in V(\mathcal{F})^{n-1}$, let*

$$I_{\mathbf{x}} = \{a \in [k] \mid (\theta(a + dk))_{d \in [n-1]} = \mathbf{x}\}.$$

If θ is well-balanced *– that is, $|I_{\mathbf{x}}| \geqslant 2|V(\mathcal{F})|^n$ for every $\mathbf{x} \in V(\mathcal{F})^{n-1}$ – then θ is an isomorphism pinning for $(\mathcal{F}, \alpha)$.*

The proof of Lemma 32, deferred to Section A, requires more sophisticated indexing but is not fundamentally different from the proof of Proposition 30. Instead of constructing instances from one, three, or two tuples $\mathbf{p}$ indexed by $V(\mathcal{F})^2 \times [t]$ in the three steps of the proof Proposition 30, we use one, n, and $n-1$ tuples $\mathbf{p}$ indexed by $\mathcal{J}(\mathcal{F})$ (recall (9)), respectively, where n is the maximum arity among the functions in $\mathcal{F}$. This accounts for possible asymmetry and distinct arities of functions in $\mathcal{F}$.

Now we remove the requirement that θ be well-balanced, which removes the requirement that k be large. The proof of the next theorem follows and generalizes the proof of [12, Theorem 3.1].

Lemma 33. *Let $(\mathcal{F}, \alpha)$ and $(\mathcal{G}, \beta)$ be finite similar domain-weighted constraint function sets with $|V(\mathcal{F})| \geqslant |V(\mathcal{G})|$ and $\mathcal{F}$ twin-free. Let $k \geqslant 0$ and $\varphi : [k] \to V(\mathcal{F})$ and $\psi : [k] \to V(\mathcal{G})$. If $(\mathcal{F}, \alpha, \varphi)$ and $(\mathcal{G}, \beta, \psi)$ are simple-#CSP-indistinguishable and there exist $\ell \geqslant k$ and an extension $\Theta : [\ell] \to V(\mathcal{F})$ of φ that is an isomorphism pinning of $(\mathcal{F}, \alpha)$, then $|V(\mathcal{F})| = |V(\mathcal{G})|$ and $(\mathcal{F}, \alpha, \varphi) \cong (\mathcal{G}, \beta, \psi)$.*

Proof. First, if $\ell = k$, then φ itself is an isomorphism pinning, and we are done. Otherwise, assume $\ell > k$. Let $E(\varphi) = \{\Phi : [\ell] \to V(\mathcal{F}) \mid \Phi \text{ extends } \varphi\}$ and $E(\psi) = \{\Psi : [\ell] \to V(\mathcal{G}) \mid \Psi \text{ extends } \psi\}$ be the sets of all extensions of φ and ψ to $[\ell]$, respectively. Define

$$A := \{\Phi \in E(\varphi) \mid \exists \sigma \in \mathrm{Aut}(\mathcal{F}, \alpha) \text{ s.t. } \Phi = \sigma \circ \Theta\} \text{ and}$$
$$B := \{\Psi \in E(\psi) \mid \exists \text{ isomorphism } \sigma \text{ between } (\mathcal{F}, \alpha) \text{ and } (\mathcal{G}, \beta) \text{ s.t. } \Psi = \sigma \circ \Theta\}.$$

We will show $B \neq \varnothing$. As Θ is an isomorphism pinning of $(\mathcal{F}, \alpha)$, if $\Phi \in E(\varphi) \setminus A$, then $(\mathcal{F}, \alpha, \Theta)$ and $(\mathcal{F}, \alpha, \Phi)$ are not simple-#CSP-indistinguishable, so there is a $K^{\Phi} \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; \ell]$ such that

$$Z_{\alpha}^{\Theta}(K^{\Phi}) \neq Z_{\alpha}^{\Phi}(K^{\Phi}). \tag{20}$$

Similarly, if $\Psi \in E(\psi) \setminus B$, then the triples $(\mathcal{F}, \alpha, \Theta)$ and $(\mathcal{G}, \beta, \Psi)$ are not simple-#CSP-indistinguishable, so there is a $K^{\Psi} \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; \ell]$ such that

$$Z_{\alpha}^{\Theta}(K^{\Psi}) \neq Z_{\beta}^{\Psi}(K^{\Psi}_{\mathcal{F}\to\mathcal{G}}). \tag{21}$$

Define the set

$$J := (E(\varphi) \setminus A) \sqcup (E(\psi) \setminus B)$$

to index these nonisomorphism witnesses, and for every choice of $\mathbf{q} := (q_{\Lambda})_{\Lambda \in J} \in [|E(\varphi) \sqcup E(\psi)|]^J = [|V(\mathcal{F})|^{\ell-k} + |V(\mathcal{G})|^{\ell-k}]^J$, define the ℓ-labeled instance product

$$K^{\mathbf{q}} := \prod_{\Lambda \in J} (K^{\Lambda})^{q_{\Lambda}} \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; \ell].$$

Then, by multiplicativity (2),

$$Z_{\alpha}^{\Phi}(K^{\mathbf{q}}) = \prod_{\Lambda \in J} \left(Z_{\alpha}^{\Phi}(K^{\Lambda})\right)^{q_{\Lambda}} \tag{22}$$

for any $\Phi \in E(\varphi)$. For any $K \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; \ell]$, define $\pi_k(K) \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; k]$ by removing the labels (but not the underlying variables) in $[\ell] \setminus [k]$ from K'. Then, for any $K \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; \ell]$,

$$\begin{aligned} &\sum_{\Phi \in E(\varphi)} \left(\prod_{m \in [\ell]\setminus[k]} \alpha_{\Phi(m)} \right) Z_{\alpha}^{\Phi}(K) = Z_{\alpha}^{\varphi}(\pi_k(K)) \\ &= Z_{\beta}^{\psi}(\pi_k(K)_{\mathcal{F}\to\mathcal{G}}) = \sum_{\Psi \in E(\psi)} \left(\prod_{m \in [\ell]\setminus[k]} \beta_{\Psi(m)} \right) Z_{\beta}^{\Psi}(K_{\mathcal{F}\to\mathcal{G}}), \end{aligned} \tag{23}$$

where the second equality holds because the triples $(\mathcal{F}, \alpha, \varphi)$ and $(\mathcal{G}, \beta, \psi)$ are simple-#CSP-indistinguishable. Substituting $K := K^{\mathbf{q}}$ in (23) and applying (22), we obtain

$$0 = \sum_{\Phi \in E(\varphi)} \left(\prod_{m \in [\ell] \setminus [k]} \alpha_{\Phi(m)} \right) \prod_{\Lambda \in J} \left(Z_\alpha^\Phi(K^\Lambda) \right)^{q_\Lambda} + \sum_{\Psi \in E(\psi)} \left(- \prod_{m \in [\ell] \setminus [k]} \beta_{\Psi(m)} \right) \prod_{\Lambda \in J} \left(Z_\beta^\Psi(K^\Lambda_{\mathcal{F} \to \mathcal{G}}) \right)^{q_\Lambda}. \tag{24}$$

Considering (24) for every choice of $\mathbf{q} \in [|E(\varphi) \sqcup E(\psi)|]^J$, we may apply Lemma 27 with

$$I := E(\varphi) \sqcup E(\psi), \;\; a_i := \begin{cases} \prod_{m \in [\ell] \setminus [k]} \alpha_{\Phi(m)} & i = \Phi \in E(\varphi) \\ - \prod_{m \in [\ell] \setminus [k]} \beta_{\Psi(m)} & i = \Psi \in E(\psi) \end{cases}$$
$$b_{i,\Lambda} := \begin{cases} Z_\alpha^\Phi(K^\Lambda) & i = \Phi \in E(\varphi) \\ Z_\beta^\Psi(K^\Lambda_{\mathcal{F} \to \mathcal{G}}) & i = \Psi \in E(\psi) \end{cases}.$$

For every K^Λ (indeed, for every $K \in \mathcal{PLI}^{\text{simp}}[\mathcal{F}; \ell]$), any $\Phi \in A$ and $\Psi \in B$ satisfy

$$b_{\Phi,\Lambda} = Z_\alpha^\Phi(K^\Lambda) = Z_\alpha^\Theta(K^\Lambda) = Z_\beta^\Psi(K_{\mathcal{F} \to \mathcal{G}}) = b_{\Psi,\Lambda}. \tag{25}$$

Thus, when we apply Lemma 27, there is a single equivalence class containing $A \sqcup B \subset I$. Furthermore, if $\Phi' \in E(\varphi) \setminus A$ and $\Phi \in A$, then, using (20) and (25) (with $\Lambda := \Phi'$),

$$b_{\Phi',\Phi'} = Z_\alpha^{\Phi'}(K^{\Phi'}) \neq Z_\alpha^\Theta(K^{\Phi'}) = b_{\Phi,\Phi'}.$$

Similarly, if $\Psi' \in E(\psi) \setminus B$ and $\Psi \in B$, then, using (21) and (25),

$$b_{\Psi',\Psi'} = Z_\beta^{\Psi'}(K^{\Psi'}_{\mathcal{F} \to \mathcal{G}}) \neq Z_\alpha^\Theta(K^{\Psi'}) = b_{\Psi,\Psi'}$$

Therefore $A \sqcup B$ constitutes an *entire* equivalence class. So, by Lemma 27,

$$\sum_{\Phi \in A} \left(\prod_{m \in [\ell] \setminus [k]} \alpha_{\Phi(m)} \right) - \sum_{\Psi \in B} \left(\prod_{m \in [\ell] \setminus [k]} \beta_{\Psi(m)} \right) = 0. \tag{26}$$

For any $\Phi \in A$, there is a $\sigma \in \operatorname{Aut}(\mathcal{F}, \alpha)$ satisfying $\Phi = \sigma \circ \Theta$. Then $\alpha_{\Phi(m)} = \alpha_{\sigma(\Theta(m))} = \alpha_{\Theta(m)}$, a value independent of the choice of Φ. So (26) becomes

$$|A|_{\mathbb{F}} \prod_{m \in [\ell] \setminus [k]} \alpha_{\Theta(m)} = \sum_{\Psi \in B} \left(\prod_{m \in [\ell] \setminus [k]} \beta_{\Psi(m)} \right), \tag{27}$$

where $|A|_{\mathbb{F}}$ is a sum of $|A|$ copies of the multiplicative identity $1_{\mathbb{F}} \in \mathbb{F}$. Each $\alpha_{\Theta(m)} \neq 0$ and, since $\mathbb{F}$ has nonzero characteristic and $A \ni \Theta$ (so $|A| > 1$) , $|A|_{\mathbb{F}} \neq 0$. Hence (27) is nonzero, so B is nonempty. Any $\Psi \in B$ extends ψ and gives an isomorphism σ between $(\mathcal{F}, \alpha)$ and $(\mathcal{G}, \beta)$ such that $\Psi = \sigma \circ \Theta$. Since Θ itself extends φ, restricting $\Psi = \sigma \circ \Theta$ to $[k]$ gives $\psi = \sigma \circ \varphi$, as desired. $\square$

Now Lemmas 32 and 33 (and Lemma 29) combine to prove the following theorem for finite $\mathcal{F}$ and $\mathcal{G}$. Then we bootstrap the finite case to $\mathcal{F}$ and $\mathcal{G}$ of arbitrary cardinality.

Theorem 34. *Let $(\mathcal{F}, \alpha)$ and $(\mathcal{G}, \beta)$ be similar domain-weighted constraint function sets with $|V(\mathcal{F})| \geqslant |V(\mathcal{G})|$, and $\mathcal{F}$ twin-free. Let $k \geqslant 0$ and $\varphi : [k] \to V(\mathcal{F})$ and $\psi : [k] \to V(\mathcal{G})$. If $(\mathcal{F}, \alpha, \varphi)$ and $(\mathcal{G}, \beta, \psi)$ are simple-#CSP-indistinguishable, then $|V(\mathcal{F})| = |V(\mathcal{G})|$ and $(\mathcal{F}, \alpha, \varphi) \cong (\mathcal{G}, \beta, \psi)$.*

Proof. First suppose $\mathcal{F}$ and $\mathcal{G}$ are finite. If all constraint functions in $\mathcal{F}$ and $\mathcal{G}$ are unary, then apply Lemma 29. Otherwise, by Lemma 33, it suffices to find an extension $\Theta : [\ell] \to V(\mathcal{F})$ of φ that is an isomorphism pinning of $(\mathcal{F}, \alpha)$. By choosing sufficiently large ℓ (no larger than $k + 2(n-1)|V(\mathcal{F})|^{2n-1}$), we can always extend φ to a well-balanced Θ, and, by Lemma 32, such a Θ is an isomorphism pinning of $(\mathcal{F}, \alpha)$. This gives the desired result for finite $\mathcal{F}$ and $\mathcal{G}$.

Next, consider $\mathcal{F}$ and $\mathcal{G}$ with arbitrary cardinality. Define the finite set

$$\Sigma = \{\sigma : V(\mathcal{F}) \to V(\mathcal{G}) \mid \sigma \text{ is a bijection and } \psi = \sigma \circ \varphi \text{ and } \alpha_i = \beta_{\sigma(i)} \text{ for all } i \in V(\mathcal{F})\}.$$

For any finite twin-free $\mathcal{F}' \subset \mathcal{F}$ and corresponding $\mathcal{G}' \subset \mathcal{G}$, $(\mathcal{F}', \alpha, \varphi)$ and $(\mathcal{G}', \beta, \psi)$ inherit the simple-#CSP-indistinguishablity of $(\mathcal{F}, \alpha, \varphi)$ and $(\mathcal{G}, \beta, \psi)$, so, by the finite case above, there is a $\sigma \in \Sigma$ that is an isomorphism of $(\mathcal{F}', \alpha, \varphi)$ and $(\mathcal{G}', \beta, \psi)$. In particular, Σ is nonempty. Suppose towards contradiction that there is no $\sigma \in \Sigma$ that is an isomorphim of the full sets $\mathcal{F}$ and $\mathcal{G}$. Then, for every $\sigma \in \Sigma$, there is a pair $\mathcal{F} \ni F_\sigma \leftrightsquigarrow G_\sigma \in \mathcal{G}$ such that σ is not an isomorphism of F_σ and G_σ. Define the finite, nonempty sets

$$\mathcal{F}' = \{F_\sigma \mid \sigma \in \Sigma\} \text{ and } \mathcal{G}' = \{G_\sigma \mid \sigma \in \Sigma\}.$$

If $\mathcal{F}'$ is not twin-free, then, for each $i, i' \in V(\mathcal{F})$ that are twins for $\mathcal{F}'$, find an $F_{i,i'} \in \mathcal{F}$ such that there exist $\mathbf{x}$ and r for which $F_{i,i'}(\mathbf{x}^{r \hookleftarrow i}) \neq F_{i,i'}(\mathbf{x}^{r \hookleftarrow i'})$ (such an $F_{i,i'}$ must exist because $\mathcal{F}$ is twin-free), and define

$$\mathcal{F}'' = \mathcal{F}' \cup \{F_{i,i'} \mid i, i' \in V(\mathcal{F}) \text{ are twins for } \mathcal{F}'\}.$$

Define $\mathcal{G}''$ to be the subset of $\mathcal{G}$ corresponding to $\mathcal{F}''$. As $\mathcal{F}''$ and $\mathcal{G}''$ are finite and $\mathcal{F}''$ is twin-free, by the finite case above, there is a $\sigma_0 \in \Sigma$ that is an isomorphism of $\mathcal{F}''$ and $\mathcal{G}''$. In particular, since $\mathcal{F}'' \ni F_{\sigma_0} \leftrightsquigarrow G_{\sigma_0} \in \mathcal{G}''$, σ_0 is an isomorphism of F_{σ_0} and G_{σ_0}, a contradiction. $\square$

Next, we introduce domain weights to unweighted constraint function sets to remove the twin-free requirement. The proof of the next corollary generalizes the proof of [12, Corollary 6.2].

Corollary 35. *Let $\mathcal{F}$ and $\mathcal{G}$ be similar constraint function sets, and let $k \geqslant 0$, $\varphi : [k] \to V(\mathcal{F})$, and $\psi : [k] \to V(\mathcal{G})$. If $(\mathcal{F}, \varphi)$ and $(\mathcal{G}, \psi)$ are simple-#CSP-indistinguishable, then $|V(\mathcal{F})| = |V(\mathcal{G})|$ and there is an isomorphism σ from $\mathcal{F}$ to $\mathcal{G}$ such that $\psi' = \sigma \circ \varphi$, where $\psi'(i)$ is a twin of $\psi(i)$ for every $i \in [k]$.*

Proof. Let $I_0, \dots, I_{s-1}$ be the partition of $V(\mathcal{F})$ into equivalence classes under the twin relation. Define the twin-contracted constraint function set $\widetilde{\mathcal{F}}$ with domain $V(\widetilde{\mathcal{F}}) = [s]$ by replacing each $F \in \mathcal{F}$ with $\widetilde{F}$ defined by $\widetilde{F}(\mathbf{y}) := F(\mathbf{x})$ for arbitrary choices of $x_i \in I_{y_i}$ for $i \in [n_F]$. Introduce domain weights α defined by $\alpha_\ell = |I_\ell|$ for $\ell \in [s]$. Define $\widetilde{\varphi} : [k] \to V(\widetilde{\mathcal{F}})$ by setting $\widetilde{\varphi}(m) = \ell$ if $\varphi(m) \in I_\ell$. Now $\widetilde{\mathcal{F}}$ is twin-free and $(\mathcal{F}, \varphi)$ and $(\widetilde{\mathcal{F}}, \alpha, \widetilde{\varphi})$ are #CSP-indistinguishable. Similarly partition $V(\mathcal{G})$ into equivalence classes $J_0, \dots, J_{s'-1}$ and define a twin-contracted $(\widetilde{\mathcal{G}}, \beta, \widetilde{\psi})$. Then, since $(\mathcal{F}, \varphi)$ and $(\mathcal{G}, \psi)$ are simple-#CSP-indistinguishable by assumption, $(\widetilde{\mathcal{F}}, \alpha, \widetilde{\varphi})$ and $(\widetilde{\mathcal{G}}, \beta, \widetilde{\psi})$ are simple-#CSP-indistinguishable. As $\widetilde{\mathcal{F}}$ is now twin-free, we may apply Theorem 34 to conclude that $s = s'$ and there is an isomorphism ξ from $(\widetilde{\mathcal{F}}, \alpha)$ to $(\widetilde{\mathcal{G}}, \beta)$ such that $\widetilde{\psi} = \xi \circ \widetilde{\varphi}$.

Define $\sigma : V(\mathcal{F}) \to V(\mathcal{G})$ as follows. For each $\ell \in [s] = V(\widetilde{\mathcal{F}})$, ξ associates $I_\ell \subset V(\mathcal{F})$ with $J_{\xi(\ell)} \subset V(\mathcal{G})$, and $|I_\ell| = \alpha_\ell = \beta_{\xi(\ell)} = |J_{\xi(\ell)}|$. Choose an arbitrary bijection between I_ℓ and $J_{\xi(\ell)}$ and have σ map I_ℓ into $J_{\xi(\ell)}$ according to this bijection. This σ satisfies the desired properties. $\square$

Finally, the $k = 0$ case of Corollary 35 is equivalent to Theorem 8, but slightly stronger because it only assumes simple indistinguishablity:

Corollary 36. *Let $\mathcal{F}$ and $\mathcal{G}$ be similar constraint function sets. Then $\mathcal{F} \cong \mathcal{G}$ if and only if $\mathcal{F}$ and $\mathcal{G}$ are simple-*#CSP*-indistinguishable.*

4.5 Constructiveness of the Interpolation Proof

For similar domain-weighted constraint function sets $(\mathcal{F}, \alpha)$ and $(\mathcal{G}, \beta)$ with $\mathcal{F}$ twin-free and $|V(\mathcal{F})| \geqslant |V(\mathcal{G})|$, and $\varphi : [k] \to V(\mathcal{F})$, $\psi : [k] \to V(\mathcal{G})$, Theorem 34 asserts that if $(\mathcal{F}, \alpha, \varphi) \ncong (\mathcal{G}, \beta, \psi)$, then there is some witness instance $K \in \mathcal{PLI}^{\text{simp}}[\mathcal{F}; k]$ such that $Z_\alpha^\varphi(K) \neq Z_\alpha^\psi(K_{\mathcal{F}\to\mathcal{G}})$. If $\mathcal{F}$ and $\mathcal{G}$ are finite, then the proofs of Lemma 32 and Lemma 33 construct an explicit finite list of instances in $\mathcal{PLI}^{\text{simp}}[\mathcal{F}; k]$ guaranteed to contain such a witness as follows (if $\mathcal{F}$ and $\mathcal{G}$ are infinite, then we cannot expect to produce such a list in bounded time). The proof of Theorem 34 first extends φ to an isomorphism pinning Θ with domain $[\ell]$, where $\ell \leqslant k + 2(n-1)|V(\mathcal{F})|^{2n-1}$ (n is the maximum arity among functions in $\mathcal{F}$). Then the proof of Lemma 33 shows that

$$Z_\alpha^\varphi(\pi_k(K^{\mathbf{q}})) = Z_\beta^\psi(\pi_k(K^{\mathbf{q}})_{\mathcal{F}\to\mathcal{G}}) \text{ for every } \mathbf{q} \in [|V(\mathcal{F})|^{\ell-k} + |V(\mathcal{G})|^{\ell-k}]^J$$

if and only if $(\mathcal{F}, \alpha, \varphi) \cong (\mathcal{G}, \beta, \psi)$. Therefore, if $(\mathcal{F}, \alpha, \varphi) \ncong (\mathcal{G}, \beta, \psi)$, then the finite set

$$\left\{\pi_k(K^{\mathbf{q}}) \mid \mathbf{q} \in [|V(\mathcal{F})|^{\ell-k} + |V(\mathcal{G})|^{\ell-k}]^J\right\}$$

is guaranteed to contain a nonisomorphism witness. Constructing this set entails constructing the instances $\{K^\Lambda \mid \Lambda \in J\}$ composing $K^{\mathbf{q}}$, which are defined existentially using (20) and (21). The proof of Lemma 32 explicitly constructs a finite set to which each K^Λ

must belong: let

$$
\begin{aligned}
W_\Theta = &\left\{K^{\mathbf{p}} \mid \mathbf{p} = [2|V(\mathcal{F})|]^{\mathcal{J}(\mathcal{F})}\right\} \\
&\cup \left\{K^{F,\mathbf{p}^{(0)},\dots,\mathbf{p}^{(n_F-1)}} \mid F \in \mathcal{F}, \mathbf{p}^{(0)},\dots,\mathbf{p}^{(n_F-1)} \in [|V(\mathcal{F})|]^{\mathcal{J}(\mathcal{F})}\right\} \\
&\cup \left\{K^{F,\mathbf{p}^{(0)},\dots,\mathbf{p}^{(n_F-2)}} \mid F \in \mathcal{F}, \mathbf{p}^{(0)},\dots,\mathbf{p}^{(n_F-2)} \in [|V(\mathcal{F})|]^{\mathcal{J}(\mathcal{F})}\right\} \subset \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F};\ell]
\end{aligned}
$$

be the (finite) set of all #CSP($\mathcal{F}$) instances whose constraint sets are defined in (28), (32), and (36), the three steps of the proof of Lemma 32 (with $\theta := \Theta$ in the statement of Lemma 32). If $\Phi \in E(\varphi) \setminus A$, then $(\mathcal{F},\alpha,\Theta) \ncong (\mathcal{F},\alpha,\Phi)$, so, by the proof of Lemma 32, there is a $K^\Phi = K^\Lambda \in W_\Theta$ satisfying (20). Similarly, if $\Psi \in E(\psi) \setminus B$, then $(\mathcal{F},\alpha,\Theta) \ncong (\mathcal{G},\beta,\Psi)$, so there is a $K^\Psi = K^\Lambda \in W_\Theta$ satisfying (21). Thus each $K^{\mathbf{q}}$ is composed of instances in the explicitly constructed set W_Θ.

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A Appendix

For convenince, we restate Lemma 32.

Lemma (Lemma 32). Let $\mathcal{F} = \{F_j \mid j \in [t]\}$ be twin-free, with domain weights α. Let $n = \max_{j\in[t]} n_j$ be the maximum arity among all functions in $\mathcal{F}$, and assume $n \geqslant 2$. Suppose $\theta : [(n-1)k] \to V(\mathcal{F})$, and for every $\mathbf{x} \in V(\mathcal{F})^{n-1}$, let

$$I_{\mathbf{x}} = \{a \in [k] \mid (\theta(a + dk))_{d\in[n-1]} = \mathbf{x}\}.$$

If θ is *well-balanced* – that is, $|I_{\mathbf{x}}| \geqslant 2|V(\mathcal{F})|^n$ for every $\mathbf{x} \in V(\mathcal{F})^{n-1}$ – then θ is an isomorphism pinning for $(\mathcal{F}, \alpha)$.

Proof. Let $(\mathcal{G}, \beta)$ be similar to $\mathcal{F}$ with $|V(\mathcal{G})| \leqslant |V(\mathcal{F})|$, and suppose $\psi : [(n-1)k] \to V(\mathcal{G})$ satisfies $Z^{\theta}_{\alpha}(K) = Z^{\psi}_{\beta}(K_{\mathcal{F}\to\mathcal{G}})$ for every $K \in \mathcal{PLI}^{\text{simp}}[\mathcal{F}; (n-1)k]$. Since each $|I_{\mathbf{x}}| \geqslant 2|V(\mathcal{F})|^n \geqslant 2|V(\mathcal{F})| \cdot |V(\mathcal{G})|^{n-1}$, by the pigeonhole principle there exists a function $s : V(\mathcal{F})^{n-1} \to V(\mathcal{G})^{n-1}$ such that for every $\mathbf{x} \in V(\mathcal{F})^{n-1}$, the set

$$J_{\mathbf{x}} := I_{\mathbf{x}} \cap \{a \in [k] \mid (\psi(a + dk))_{d\in[n-1]} = s(\mathbf{x})\}$$

satisfies $|J_{\mathbf{x}}| \geqslant 2|V(\mathcal{F})|$. For every $\mathbf{x} \in V(\mathcal{F})^{n_j-1}$ with $n_j < n$, choose an arbitrary $\mathbf{x}' \in V(\mathcal{F})^{n-1}$ extending $\mathbf{x}$ (i.e. such that $x'_d = x_d$ for every $d \in [n_j - 1]$) and define $J_{\mathbf{x}} := J_{\mathbf{x}'}$.

Consider the $(n-1)k$-labeled variable set

$$V_1 = \{v\} \cup \{u^{(d)}_a\}_{a\in[k],d\in[n-1]},$$

where $u^{(d)}_a$ is labeled $a + dk$. For each choice of $\mathbf{p} = (p_{j\,\mathbf{x}\,r})_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})} \in [2|V(\mathcal{F})|]^{\mathcal{J}(\mathcal{F})}$ (recall (9)), construct a set $C^{\mathbf{p}}(v)$ of constraints on V_1 as follows. Choose an arbitrary $P_{j\,\mathbf{x}\,r} \subset J_{\mathbf{x}}$ with $|P_{j\,\mathbf{x}\,r}| = p_{j\,\mathbf{x}\,r}$ for each $(j, \mathbf{x}, r) \in \mathcal{J}(\mathcal{F})$ and define

$$C^{\mathbf{p}}(v) = \bigcup_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})} \bigcup_{a\in P_{j\,\mathbf{x}\,r}} \Big(F_j, \big(u^{(d)}_a\big)^{r\leftarrow\!\!\!\hookrightarrow v}_{d\in[n_j-1]}\Big). \tag{28}$$

Then define an $(n-1)k$-labeled #CSP($\mathcal{F}$) instance $K^{\mathbf{p}} = (V_1, C^{\mathbf{p}}(v)) \in \mathcal{PLI}^{\text{simp}}[\mathcal{F}; (n-1)k]$. If $a \in P_{j\,\mathbf{x}\,r} \subset J_{\mathbf{x}}$ then $\theta(a + dk) = x_d$ and $\psi(a + dk) = s(\mathbf{x})_d$ for all $d \in [n_j - 1]$. Hence the variable $u^{(d)}_a$ takes value x_d and $s(\mathbf{x})_d$ under θ and ψ, respectively, for $d \in [n_j - 1]$. These values are independent of the choice of a within $P_{j\,\mathbf{x}\,r}$. Therefore $Z^{\theta}_{\alpha}(K^{\mathbf{p}}) = Z^{\psi}_{\beta}(K^{\mathbf{p}}_{\mathcal{F}\to\mathcal{G}})$ is equivalent to

$$\sum_{i\in V(\mathcal{F})} \alpha_i \prod_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})} F_j\big(\mathbf{x}^{r\leftarrow\!\!\!\hookrightarrow i}\big)^{p_{j\,\mathbf{x}\,r}} + \sum_{i\in V(\mathcal{G})} (-\beta_i) \prod_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})} G_j\big(s(\mathbf{x})^{r\leftarrow\!\!\!\hookrightarrow i}\big)^{p_{j\,\mathbf{x}\,r}} = 0. \tag{29}$$

The sums over i correspond to the choice of assignment for the free variable v in $K^{\mathbf{p}}$ and $K^{\mathbf{p}}_{\mathcal{F}\to\mathcal{G}}$, respectively. Overall, the LHS of (29) is a sum over $V(\mathcal{F}) \sqcup V(\mathcal{G})$, with $|V(\mathcal{F}) \sqcup$

$V(\mathcal{G})| = |V(\mathcal{F})| + |V(\mathcal{G})| \leqslant 2|V(\mathcal{F})|$. Therefore, by constructing $K^{\mathbf{p}}$ and considering (29) for every choice of $\mathbf{p} \in [2|V(\mathcal{F})|]^{\mathcal{J}(\mathcal{F})}$, we may apply Lemma 27 with

$$I := V(\mathcal{F}) \sqcup V(\mathcal{G}),\ J := \mathcal{J}(\mathcal{F}),\ a_i := \begin{cases} \alpha_i & i \in V(\mathcal{F}) \\ -\beta_i & i \in V(\mathcal{G}) \end{cases},$$

$$b_{i,j\,\mathbf{x}\,r} := \begin{cases} F_j\big(\mathbf{x}^{r \hookleftarrow i}\big) & i \in V(\mathcal{F}) \\ G_j\big(s(\mathbf{x})^{r \hookleftarrow i}\big) & i \in V(\mathcal{G}) \end{cases}.$$

Since $\mathcal{F}$ is twin-free, the tuples $\big(F_j\big(\mathbf{x}^{r \hookleftarrow i}\big)\big)_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})}$ are pairwise distinct for $i \in V(\mathcal{F})$. Hence no equivalence class contains more than one element of $V(\mathcal{F})$. However, every $\alpha_i \neq 0$, so no equivalence class consists of only a single element of $V(\mathcal{F})$. Thus there is a function $\sigma : V(\mathcal{F}) \to V(\mathcal{G})$ such that $i \sim \sigma(i)$ for every $i \in V(\mathcal{F})$ – that is,

$$\big(F_j\big(\mathbf{x}^{r \hookleftarrow i}\big)\big)_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})} = \big(G_j\big(s(\mathbf{x})^{r \hookleftarrow \sigma(i)}\big)\big)_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})} \text{ for every } i \in V(\mathcal{F}). \tag{30}$$

Since no two elements of $V(\mathcal{F})$ are in the same equivalence class, σ is injective, hence bijective, as $|V(\mathcal{F})| \geqslant |V(\mathcal{G})|$. Therefore $|V(\mathcal{F})| = |V(\mathcal{G})|$, and Lemma 27 gives

$$\alpha_i = \beta_{\sigma(i)} \text{ for } i \in V(\mathcal{F}). \tag{31}$$

Next, define another family of #CSP($\mathcal{F}$) instances as follows. Fix $\mathcal{F} \ni F \leftrightsquigarrow G \in \mathcal{G}$ with common arity $n_F \leqslant n$, and let

$$V_2 := V_1 \setminus \{v\} \cup \{v_h \mid h \in [n_F]\}.$$

For $\mathbf{p}^{(0)}, \ldots, \mathbf{p}^{(n_F-1)} \in [|V(\mathcal{F})|]^{\mathcal{J}(\mathcal{F})}$, define the following set of constraints on V_2 (recall (28)):

$$C^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-1)}} := \{(F, v_0, \ldots, v_{n_F-1})\} \cup \bigcup_{h\in[n_F]} C^{\mathbf{p}^{(h)}}(v_h). \tag{32}$$

Define the labeled instance $K^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-1)}} := (V_2, C^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-1)}}) \in \mathcal{PLI}^{\mathrm{simp}}[\mathcal{F}; (n-1)k]$. Then the assumption $Z_\alpha^\theta\big(K^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-1)}}\big) = Z_\beta^\psi\big(K_{\mathcal{F}\to\mathcal{G}}^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-1)}}\big)$ is equivalent to

$$\begin{aligned} 0 = &\sum_{\mathbf{i}\in V(\mathcal{F})^{n_F}} \left(\prod_{h\in[n_F]} \alpha_{i_h}\right) F(\mathbf{i}) \prod_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F}),h\in[n_F]} F_j\big(\mathbf{x}^{r \hookleftarrow i_h}\big)^{p^{(h)}_{j\,\mathbf{x}\,r}} \\ &+ \sum_{\mathbf{i}\in V(\mathcal{G})^{n_F}} \left(-\prod_{h\in[n_F]} \beta_{i_h}\right) G(\mathbf{i}) \prod_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F}),h\in[n_F]} G_j\big(s(\mathbf{x})^{r \hookleftarrow i_h}\big)^{p^{(h)}_{j\,\mathbf{x}\,r}}, \end{aligned}$$

where the sums over $\mathbf{i}$ corresponds to the choice of assignment for the free variables $v_0, \ldots, v_{n_F-1}$. Applying (31) and (30) then gives

$$\sum_{\mathbf{i}\in V(\mathcal{F})^{n_F}} \left(\prod_{h\in[n_F]} \alpha_{i_h}\right) \big(F(\mathbf{i}) - G(\sigma(\mathbf{i}))\big) \prod_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F}),h\in[n_F]} F_j\big(\mathbf{x}^{r \hookleftarrow i_h}\big)^{p^{(h)}_{j\,\mathbf{x}\,r}} = 0. \tag{33}$$

Considering $K^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-1)}}$ and (33) for every $\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-1)} \in [|V(\mathcal{F})|]^{\mathcal{J}(\mathcal{F})}$, we may apply Corollary 28 with

$$m := n_F,\ J = \mathcal{J}(\mathcal{F}),\ a_{\mathbf{i}} := \left(\prod_{h\in[n_F]} \alpha_{i_h}\right)\big(F(\mathbf{i}) - G(\sigma(\mathbf{i}))\big),$$
$$b_{i,j\,\mathbf{x}\,r} := F_j\big(\,\mathbf{x}^{r\hookleftarrow i}\,\big),\ p_{h,j\,\mathbf{x}\,r} := p^{(h)}_{j\,\mathbf{x}\,r}.$$

Again, by twin-freeness, the tuples $\big(F_j\big(\,\mathbf{x}^{r\hookleftarrow i}\,\big)\big)_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})}$ are distinct for distinct $i \in V(\mathcal{F})$, so the larger tuples $\big(F_j\big(\,\mathbf{x}^{r\hookleftarrow i_h}\,\big)\big)_{h\in[n_F],(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F})}$ are distinct for distinct $\mathbf{i} \in V(\mathcal{F})^{n_F}$. Corollary 28 asserts that, for all $\mathbf{i} \in V(\mathcal{F})^{n_F}$, $(\prod_{h=1}^{n_F} \alpha_{i_h})\,(F(\mathbf{i}) - G(\sigma(\mathbf{i}))) = 0$. Since each $\alpha_i \neq 0$ and our choice of F and G was arbitrary, this implies

$$F(\mathbf{i}) = G(\sigma(\mathbf{i})) \text{ for every } \mathbf{i} \in V(\mathcal{F})^{n_F} \text{ and every pair } \mathcal{F} \ni F \leftrightsquigarrow G \in \mathcal{G}\,. \tag{34}$$

Combined with (31), (34) implies that σ is a domain-weighted isomorphism of $(\mathcal{F},\alpha)$ and $(\mathcal{G},\beta)$.

It remains to show that $\psi = \sigma \circ \theta$. Again let $\mathcal{F} \ni F \leftrightsquigarrow G \in \mathcal{G}$, with common arity n_F. Fix $c \in [(n-1)k]$. If $n_F = 1$, let $K \in \mathcal{PLI}^{\text{simp}}[\mathcal{F};(n-1)k]$ be an instance with no unlabeled/free variables and a single constraint (F, v_c), where v_c is the variable labeled c. Then

$$F(\theta(c)) = Z^{\theta}_{\alpha}(K) = Z^{\psi}_{\beta}(K_{\mathcal{F}\to\mathcal{G}}) = G(\psi(c)). \tag{35}$$

Otherwise, if $n_F \geqslant 2$, define a third family of #CSP($\mathcal{F}$) instances as follows. Define

$$V_3 := V_2 \setminus \{v_{n_F-1}\} = V_1 \cup \{v_h \mid h \in [n_F-1]\}.$$

Write $c = a_c + d_c k$ (so that $u^{(d_c)}_{a_c}$ is labeled c). Fix $\rho \in [n_F]$. For $\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-2)} \in [|V(\mathcal{F})|]^{\mathcal{J}(\mathcal{F})}$, define the following set of constraints on V_2:

$$C^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-2)}} := \{(F, v_0,\ldots v_{\rho-1}, u^{(d_c)}_{a_c}, v_\rho,\ldots,v_{n_F-2})\} \cup \bigcup_{h\in[n_F-1]} C^{\mathbf{p}^{(h)}}(v_h). \tag{36}$$

Define the instance $K^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-2)}} := (V_3, C^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-2)}}) \in \mathcal{PLI}^{\text{simp}}[\mathcal{F};(n-1)k]$. Now the assumption $Z^{\theta}_{\alpha}\big(K^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-2)}}\big) = Z^{\psi}_{\beta}\big(K^{F,\mathbf{p}^{(0)},\ldots,\mathbf{p}^{(n_F-2)}}_{\mathcal{F}\to\mathcal{G}}\big)$ is equivalent to

$$0 = \sum_{\mathbf{i}\in V(\mathcal{F})^{n_F-1}} \left(\prod_{h\in[n_F-1]} \alpha_{i_h}\right) F\big(\,\mathbf{i}^{\rho\hookleftarrow\theta(c)}\,\big) \prod_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F}),h\in[n_F-1]} F_j\big(\,\mathbf{x}^{r\hookleftarrow i_h}\,\big)^{p^{(h)}_{j\,\mathbf{x}\,r}}$$
$$+ \sum_{\mathbf{i}\in V(\mathcal{G})^{n_F-1}} \left(-\prod_{h\in[n_F-1]} \beta_{i_h}\right) G\big(\,\mathbf{i}^{\rho\hookleftarrow\psi(c)}\,\big) \prod_{(j,\mathbf{x},r)\in\mathcal{J}(\mathcal{F}),h\in[n_F-1]} G_j\big(s(\mathbf{x})^{r\hookleftarrow i_h}\big)^{p^{(h)}_{j\,\mathbf{x}\,r}}.$$

Applying (31) and (30) gives

$$0 = \sum_{\mathbf{i} \in V(\mathcal{F})^{n_F - 1}} \left(\prod_{h \in [n_F - 1]} \alpha_{i_h} \right) \left(F\left(\mathbf{i}^{\rho \hookleftarrow \theta(c)} \right) - G\left(\sigma(\mathbf{i})^{\rho \hookleftarrow \psi(c)} \right) \right)$$
$$\cdot \prod_{(j, \mathbf{x}, r) \in \mathcal{J}(\mathcal{F}), h \in [n_F - 1]} F_j\left(\mathbf{x}^{r \hookleftarrow i_h} \right)^{p^{(h)}_{j\,\mathbf{x}\,r}}.$$

As above, $\left(F_j\left(\mathbf{x}^{r \hookleftarrow i_h}\right)\right)_{h \in [n_F - 1], (j, \mathbf{x}, r) \in \mathcal{J}(\mathcal{F})}$ are distinct for distinct $\mathbf{i} \in V(\mathcal{F})^{n_F - 1}$. Hence by a similar application of Corollary 28 with $m := n_F - 1$, we have $F\left(\mathbf{i}^{\rho \hookleftarrow \theta(c)}\right) = G\left(\sigma(\mathbf{i})^{\rho \hookleftarrow \psi(c)}\right)$ for all $\mathbf{i} \in V(\mathcal{F})^{n_F - 1}$. This holds for any pair $F \leftrightsquigarrow G$ (with unary F and G handled by (35)) and any $\rho \in [n_F]$. Hence, for all $(j, \mathbf{i}, \rho) \in \mathcal{J}(\mathcal{F})$,

$$F_j\left(\mathbf{i}^{\rho \leftarrow \theta(c)}\right) = G_j\left(\sigma(\mathbf{i})^{\rho \leftarrow \psi(c)}\right) = F_j\left(\mathbf{i}^{\rho \leftarrow \sigma^{-1}(\psi(c))}\right),$$

where the second equality is (34). Since $\mathcal{F}$ is twin-free, we have $\theta(c) = \sigma^{-1}(\psi(c))$, hence $\sigma(\theta(c)) = \psi(c)$. We chose $c \in [(n-1)k]$ arbitrarily, so $\psi = \sigma \circ \theta$. $\square$