THE UNIVERSITY OF CHICAGO

COHERENT CONFIGURATIONS: MOTION, SPECTRAL PROPERTIES, ROBUSTNESS

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ABSTRACT

The principal theme of this thesis is the interplay between symmetry and regularity in discrete structures. The most general class of structures we consider are *coherent configurations*, certain highly regular colorings of complete graphs. This class includes such diverse structures as the orbital configurations of permutation groups and association schemes originating from the design of experiments in statistics. Metric schemes, a subclass of association schemes, are derived from distance-regular graphs. Johnson, Hamming, and Grassman schemes are special classes of great importance among metric schemes. We study structural and spectral properties of coherent configurations with special attention to the subclasses mentioned. As a culmination of this analysis, we confirm Babai's conjecture on the minimal degree of the automorphism group for distance-regular graphs of bounded diameter and for primitive coherent configurations of rank 4.

The minimal degree of a permutation group G is the minimum number of points not fixed by non-identity elements of G. Lower bounds on the minimal degree have strong structural consequences on G. Babai conjectured that for some constant c > 0 the automorphism group of a primitive coherent configuration on n vertices has minimal degree $\geq cn$ with known exceptions¹. If confirmed, this conjecture gives a CFSG²-free proof of the Liebeck-Saxl classification of primitive groups with sublinear minimal degree. Moreover, if confirmed, this conjecture would point to potential simplification of some steps in Babai's quasipolynomialtime algorithm for the Graph Isomorphism problem.

In this thesis we confirm Babai's conjecture for distance-regular graphs (metric schemes) of bounded diameter and for primitive coherent configurations of rank 4.

Central to our approach is the study of spectral parameters of distance-regular graphs,

^{1.} Recent work by Sean Eberhard expanded the class of known exceptions, but (i) it does not affect the implication in the next sentence about CFSG-free proof of the Liebeck-Saxl classification; (ii) the conjecture for distance-regular graphs is not affected.

^{2.} Classification of Finite Simple Groups

such as spectral gap and smallest eigenvalue.

The spectral gap of a graph is known to be tightly related to expansion properties of the graph. Hence, lower bounds on the spectral gap are widely applicable in various areas of mathematics and theoretical computer science. In this thesis we prove that a distanceregular graph with a dominant distance is a spectral expander. Our lower bound on the spectral gap depends only on the diameter of the graph. The key ingredient of the proof is a new inequality on the intersection numbers.

At the same time, graphs of which the smallest eigenvalue has small absolute value are known to enjoy a rich geometric structure (see, e.g., celebrated results of Hoffman, Seidel, Neumaier, and Cameron et al.).

In this thesis we characterize Hamming graphs as distance-regular graphs of diameter d with smallest eigenvalue -d and $^{3} \mu \leq 3$, under mild additional assumptions.

We also characterize Johnson and Hamming graphs as geometric distance-regular graphs satisfying certain inequality constraints on the spectral gap and the smallest eigenvalue. Classical characterizations of Hamming graphs H(d, q) assume equality constraints on certain parameters such as the assumption $\theta_1 = b_1 - 1$ on the second largest eigenvalue or the assumption $n = (\lambda + 2)^d$ on the number of vertices (see, e.g., results of Enomoto and Egawa). The principal novelty of our result is that we make no such tight assumptions.

Finally, in this thesis we study robustness properties of certain classes of coherent configurations. For instance, we show that the family of Johnson schemes is robust in the following sense. If a homogeneous coherent configuration \mathfrak{X} on n vertices or its fission contains a Johnson scheme J(s,d) as a subconfiguration on at least 5n/6 vertices and $s > 250d^4$, then \mathfrak{X} itself is a Johnson scheme. This result strengthen a 1972 theorem of Kaluzhnin and Klin that corresponds to the case where the subconfiguration itself has n vertices.

Our result is also related to Babai's "Split-or-Johnson lemma" and in particular to the

^{3.} Here μ denotes the number of common neighbours of (every) pair of vertices at distance 2.

philosophy in the theory of Graph Isomorphism testing that we can either find structure or find efficiently verifiable asymmetry. The result represents a step in the direction of simplifying the conclusion of the "Split-or-Johnson" lemma.

We also show that similar robustness results hold for Hamming and Grassmann schemes.

CHAPTER 1 INTRODUCTION

1.1 Symmetry vs. Regularity

A central theme of this thesis is the interplay between symmetry and regularity in combinatorial structures, a subject that has been studied for several decades. The "Symmetry vs. Regularity" framework builds bridges between Group Theory and Combinatorics. Additionally, the framework is related to multiple developments in Theoretical Computer Science, including Babai's quasipolynomial-time Graph Isomorphism test (Babai [2016a,b]) and the study of the complexity of the matrix multiplication (Cohn and Umans [2003, 2013]). Families of coherent configurations which naturally arise in the "Symmetry vs. Regularity" framework, such as the Johnson schemes or the Hamming schemes, due to their nice properties, also arise in numerous other contexts. For instance, Meka et al. [2015] used the eigenspaces of the Johnson schemes in the context of the planted clique problem and the "Sum-of-Squares" hierarchy. Recent progress on the Unique Games conjecture is closely related to the study of the expansion properties of Johnson and Grassmann schemes (Khot et al. [2018], Bafna et al. [2020], Hopkins et al. [2020], Dinur et al. [2021]).

In the "Symmetry vs. Regularity" framework one aims to transition from studying symmetry conditions, such as distance-transitivity, to regularity conditions, such as distanceregularity. This transition is desirable as symmetry is a global, hard-to-detect property of an object, while regularity is local and is usually easy to test. In the opposite direction, one may hope to apply Group Theory to algorithmic and combinatorial problems. For instance, the central piece of Babai's Graph Isomorphism test is a group-theoretic "Unaffected Stabilizer Theorem" which relies on the Classification of Finite Simple Groups (CFSG) through Schreier's Hypothesis.

The vehicle for this transition is *Coherent Configurations* (CCs) which are highly regular

colorings of the edges of the complete directed graphs. They were first introduced by I. Schur [1933] who used them to study permutation groups through their orbital configurations. Later, Bose and Shimamoto [1952] studied a special class of coherent configurations, called *association schemes*, in connection with combinatorial designs. Coherent configurations in their full generality were independently introduced by Weisfeiler and Leman [1968] (see Weisfeiler [1976]), and D. Higman [1967, 1970]. Higman developed the representation theory of coherent configurations and applied it to permutation groups. At the same time, a related algebraic theory of coherent configurations, called "cellular algebras," was introduced by Weisfeiler and Leman, motivated by the algorithmic problems of Graph Isomorphism and Graph Canonization. Special classes of association schemes such as strongly regular graphs and, more generally, distance-regular graphs have been the subject of intensive study in algebraic combinatorics.

A combinatorial study of coherent configurations was initiated by Babai [1981]. Coherent configurations play an important role in the study of the Graph Isomorphism problem, adding combinatorial divide-and-conquer tools to the arsenal. This approach was used by Babai [2016a,b]. Also, recently, the representation theory of coherent configurations found applications to the complexity of matrix multiplication in the work of Cohn and Umans [2013].

Let Ω be a finite set. A permutation group $G \leq \text{Sym}(\Omega)$ defines an equivalence relation on $\Omega \times \Omega$ by $(x, y) \sim (gx, gy)$ for $x, y \in \Omega$ and $g \in G$. This relation can be viewed as a coloring \mathfrak{c} of the pairs $(x, y) \in \Omega$ in which two pairs have the same color if and only if they belong to the same orbit of the induced action of G on $\Omega \times \Omega$. It is not hard to see that \mathfrak{c} has several simple combinatorial properties; these have been abstracted by Schur to define a purely combinatorial object.

Definition 1.1.1. Let Ω be a finite set. A pair $\mathfrak{X} = (\Omega, \mathfrak{c})$ is called a *coherent configuration* (*CC*) if the coloring $\mathfrak{c} : \Omega \times \Omega \to \{\text{colors}\}$ has the following properties.

(i)
$$\mathfrak{c}(x,y) \neq \mathfrak{c}(z,z)$$
 for all $x, y, z \in \Omega$ with $x \neq y$ ("edge-colors" \neq "vertex-colors").

- (ii) The color of the pair (x, y) uniquely defines the color of (y, x), for all $(x, y) \in \Omega \times \Omega$.
- (iii) for all colors i, j, t there is an *intersection number* $p_{i,j}^t$ such that, for all $u, v \in \Omega$, if $\mathbf{c}(u, v) = t$, then there exist exactly $p_{i,j}^t$ vertices $w \in \Omega$ with $\mathbf{c}(u, w) = i$ and $\mathbf{c}(w, v) = j$.

The rank of a CC is the number of (non-empty) color classes defining it.

The coherent configurations defined by the group action of $G \leq \text{Sym}(\Omega)$ on $\Omega \times \Omega$, as described above, are called *Schurian configurations*. We note that not all coherent configurations are Schurian, i.e., a coloring \mathfrak{c} satisfying (i)-(iii) may not have any group action defining it.

A coherent configuration $\mathfrak{X} = (\Omega, \mathfrak{c})$ is called *homogeneous* if $\mathfrak{c}(x) = \mathfrak{c}(y)$ for all $x, y \in \Omega$, and it is called an *association scheme* if $\mathfrak{c}(x, y) = \mathfrak{c}(y, x)$ for all $x, y \in \Omega$. A coherent configuration is called *primitive* if the digraph defined by every edge color is weakly connected.

We will be especially interested in a special well-studied case of coherent configurations, (Ω, \mathfrak{c}) , in which $\mathfrak{c}(x, y) = i$ if x and y are at distance i in the graph defined by edges of color 1. Such coherent configurations are called *metric schemes* and the corresponding color-1 graph is called a *distance-regular graph* (DRG).

We say that a coherent configuration of rank 2 is *trivial*.

1.2 Babai's conjectures on primitive coherent configurations

1.2.1 Cameron's classification of primitive permutation groups

Many questions on permutation groups reduce to the case of primitive permutation groups.

Definition 1.2.1. A permutation group $G \leq \text{Sym}(\Omega)$ is called *transitive* if for all $x, y \in \Omega$ there exists an element $g \in G$ that maps x to y.

Definition 1.2.2. A primitive permutation group is a non-trivial transitive permutation

group whose only invariant partitions are trivial (the entire set, and the partition into singletons).

Relying on the Classification of Finite Simple Groups (CFSG), Cameron [1981] classified all primitive permutation groups whose order is at least $n^{c\log n}$ for some c > 0(see Chapter 4). He showed that such groups G act on $\binom{[k]}{t}^{\ell}$ for some t, k, ℓ and satisfy $\left(A_k^{(t)}\right)^{\ell} \leq G \leq S_k^{(t)} \wr S_{\ell}$ (with the product action). Here, $A_k^{(t)}$ and $S_k^{(t)}$ are the alternating group A_k and the symmetric group S_k acting on $\binom{[k]}{t}$. Such primitive groups G are called *Cameron groups*.

In the wake of Cameron's classification, Babai initiated several projects with the aim of finding combinatorial relaxations of Cameron's results. Babai conjectured several such relaxations in terms of key parameters of permutation groups: order, minimal degree, thickness.

1.2.2 Minimal degree of a permutation group. Liebeck-Saxl's classification

One of the key contributions of this thesis confirms Babai's conjecture on the minimal degree for metric schemes of bounded rank (corresponding to distance-regular graphs of bounded diameter) and for coherent configurations of rank 4. (Babai settled the rank-3 case which corresponds to strongly regular graphs.)

Let σ be a permutation of a set Ω . The number of points not fixed by σ is called the *degree* of the permutation σ . Let G be a permutation group on the set Ω . The minimum of the degrees of non-identity elements in G is called the *minimal degree*¹ of G and is denoted by mindeg(G). One of the classical problems in the theory of permutation groups is to classify the primitive permutation groups whose minimal degree is small (see Wielandt [1964]). The study of minimal degree goes back to works of Jordan [1871] and Bochert [1892] in 19th century. In particular, Bochert [1892] proved that a doubly transitive permutation group of

^{1.} For the identity permutation group on the set Ω , we define its minimal degree to be ∞ , i.e., the minimum of the empty set.

degree n has minimal degree $\geq n/4 - 1$ with trivial exceptions.

Lower bounds on the minimal degree of a group imply strong constraints on the structure of the group. A result of Wielandt [1934] shows that a linear (in $|\Omega|$) lower bound on mindeg(G) implies a logarithmic upper bound on the degree of every alternating group involved in G as a quotient of a subgroup (see Theorem 4.3.1).

Similarly to Cameron's classification of large primitive permutation groups, using CFSG, Liebeck [1984], Liebeck and Saxl [1991] characterized primitive permutation groups of degree n with minimal degree < n/3 (see Theorem 4.2.2). In fact, they showed that those are Cameron groups.

1.2.3 Babai's combinatorial relaxations of Liebeck-Saxl's and Cameron's classifications

We define *Cameron schemes* as Schurian configurations obtained from Cameron groups. Below we discuss the combinatorial relaxation of the Liebeck-Saxl classification conjectured by Babai.

Definition 1.2.3. Following Russell and Sundaram [1998], for a combinatorial structure \mathcal{X} we use term *motion* to refer to the minimal degree of the automorphism group Aut(\mathcal{X}):

$$motion(\mathcal{X}) = mindeg(Aut(\mathcal{X})).$$
(1.1)

For distance-regular graphs Babai conjectured the following relaxation of the Liebeck-Saxl classification.

Conjecture 1.2.4 (Babai). There exists $\gamma > 0$ such that for every primitive distance-regular graph X of diameter d on n vertices either

$$motion(X) \ge \gamma n,$$

or X is a Johnson graph, or a Hamming graph, or their complement.

Babai confirmed this conjecture for distance-regular graphs of diameter ≤ 2 (i.e., for connected strongly regular graphs).

Theorem 1.2.5 (Babai [2014, 2015]). For every primitive distance-regular graph X of diameter 2 on $n \ge 29$ vertices either

$$motion(X) \ge n/8,$$

or X, or its complement, is a Johnson graph J(s, 2) or a Hamming graph H(2, s).

In this thesis we confirm this conjecture for distance-regular graphs of bounded diameter.

Theorem 1.2.6 (Main I). For every $d \ge 3$ there exists $\gamma_d > 0$, such that for every primitive distance-regular graph X of diameter d on n vertices either

$$motion(X) \ge \gamma_d n$$
,

or X is a Johnson graph, or a Hamming graph.

We prove this theorem in Chapter 8. Additionally, we show that if the primitivity assumption is dropped then one more family of exceptions arises, the family of crown graphs (see Theorem 8.4.1).

In the general case, Babai made the following conjecture.

Conjecture 1.2.7 (Babai). There exists $\gamma > 0$ such that for every primitive coherent configuration \mathfrak{X} on *n* vertices either

$$\mathrm{motion}(\mathfrak{X}) \geq \gamma n,$$

or \mathfrak{X} is a Cameron scheme.

For primitive coherent configurations of rank 3 this conjecture follows from Theorem 1.2.5 and Babai [1981]. In this thesis we confirm this conjecture for rank-4 primitive coherent configurations. However, as we discuss below, recently Eberhard [2022] found a counterexample of rank 28 and suggested a slightly modified version of Conjecture 1.2.7 (see Conj. 1.2.13).

Theorem 1.2.8 (Main II). There exists an absolute constant $\gamma_4 > 0$ such that for every primitive coherent configuration \mathfrak{X} of rank 4 on n vertices either

$$\operatorname{motion}(\mathfrak{X}) \geq \gamma_4 n_1$$

or \mathfrak{X} is a Johnson scheme, or a Hamming scheme.

This theorem is proved in Chapter 9 (see Theorem 9.5.1).

A version of Conjecture 1.2.7 in terms of the order of a group says that Cameron schemes are the only primitive coherent configurations with more than quasipolynomial number of automorphisms. A slightly weaker version has the following form.

Conjecture 1.2.9 (Babai). Let $\varepsilon > 0$. Primitive coherent configurations, other than Cameron schemes, have at most $\exp(O(n^{\varepsilon}))$ automorphisms.

The first step towards this conjecture was made by Babai [1981]. He proved that a non-trivial primitive coherent configuration on n vertices has at most $\exp(O(n^{1/2}\log^2 n))$ automorphisms. As a byproduct, he solved a then 100-year-old problem on primitive, but not doubly transitive groups, giving a nearly tight bound on their order. After more than 30 years, Sun and Wilmes [2015a,b] made the second step, proving that the only non-trivial primitive coherent configurations on n vertices that have more than $\exp(O(n^{1/3}\log^{7/3} n))$ automorphisms are Johnson and Hamming schemes.

1.2.4 Eberhard's version of Babai's conjectures

In a recent surprising result, Eberhard showed that in fact Conjectures 1.2.9 and 1.2.7 do not hold as stated. His result does not affect Conjecture 1.2.4, Conjecture 1.2.7 for configurations of rank at most 7, and Conjecture 1.2.9 for $\varepsilon > 1/8$.

Theorem 1.2.10 (Eberhard [2022]). For each $m \ge 3$, there is a non-schurian primitive association scheme \mathfrak{X} of rank 28 on $n = m^8$ vertices, such that $\operatorname{Aut}(\mathfrak{X})$ is imprimitive and $|\operatorname{Aut}(\mathfrak{X})| \ge \exp(n^{1/8}).$

However, Eberhard [2022] proposed a variant of Conjectures 1.2.9 and 1.2.7 that may still hold.

Definition 1.2.11. We say that a configuration $\mathfrak{Y} = (\Omega, \mathfrak{c}_{\mathfrak{Y}})$ is a *fusion* of a configuration $\mathfrak{X} = (\Omega, \mathfrak{c}_{\mathfrak{X}})$ if there is a map η : Range $(\mathfrak{c}_{\mathfrak{X}}) \to \text{Range}(\mathfrak{c}_{\mathfrak{Y}})$ such that $\mathfrak{c}_{\mathfrak{Y}}(u, v) = \eta(\mathfrak{c}_{\mathfrak{X}}(u, v))$ for all $u, v \in \Omega$. In this case, \mathfrak{X} is called a *fission* of \mathfrak{Y} .

For configurations \mathfrak{X} and \mathfrak{X}' on Ω , define a partial order by writing $\mathfrak{X} \preceq \mathfrak{X}'$ if \mathfrak{X} is a fission of \mathfrak{X}' .

Definition 1.2.12. A primitive coherent configuration \mathfrak{Y} defined on $\binom{[m]}{k}^d$ is called a *Cameron sandwich* if

$$\mathfrak{X}\left(\left(A_m^{(k)}\right)^d\right) \preceq \mathfrak{Y} \preceq \mathfrak{X}\left(S_m^{(k)} \wr S_d\right).$$

Conjecture 1.2.13 (Eberhard's version of Babai's conjecture). There exist $c, \gamma > 0$, such that for every primitive coherent configuration \mathfrak{X} on n vertices either

$$|\operatorname{Aut}(\mathfrak{X})| \le \exp(\log^c n) \quad and \quad \operatorname{motion}(\mathfrak{X}) \ge \gamma n,$$
(1.2)

or \mathfrak{X} is a Cameron sandwich.

Remark 1.2.14. If confirmed, Conjecture 1.2.13 would still provide a CFSG-free proof of the Cameron classification and the Liebeck-Saxl classification. Additionally, if confirmed, it

would point to potential simplification of Babai's quasipolynomial Graph Isomorphism test as mentioned in [Babai, 2016b, Remark 6.1.3].

1.3 Robustness of coherent configurations

1.3.1 Individualization and refinement

In algorithmic applications, the interplay between symmetry and regularity frequently arises in the context of *individualization/refinement* technique. This is a standard and widely used practical technique for solving tasks related to symmetry computations of graphs and other combinatorial objects, which include computing automorphism groups, isomorphism tests, canonical labeling tools. In particular, individualization/refinement is central to Babai's Graph Isomorphism test (Babai [2016a,b]).

In this technique, one breaks the symmetry of, say, a graph by assigning unique colors to a small subset of its vertices (*individualization*). After that, one propagates the asymmetry, created by individualizing these vertices, using a refinement step.

A classical example of a refinement was introduced by Weisfeiler and Leman [1968]. The Weisfeiler-Leman refinement proceeds in rounds. In each round it takes a configuration $\mathfrak{X} = (\Omega, \mathfrak{c})$ of rank r and for each pair $(x, y) \in \Omega \times \Omega$ it encodes in a new color $\mathfrak{c}'(x, y)$ the following information: the color $\mathfrak{c}(x, y)$, and for every $i, j \leq r$ the number of vertices z with $\mathfrak{c}(x, z) = i, \mathfrak{c}(z, y) = j$. It is easy to see that for the refined coloring \mathfrak{c}' , the structure $\mathfrak{X}' = (\Omega, \mathfrak{c}')$ is a configuration as well. The refinement process applied to a configuration \mathfrak{X} takes \mathfrak{X} as an input on the first round, and on every subsequent round in takes as an input the output of the previous round. The refinement process stops when it reaches a stable configuration (i.e, $\mathfrak{Y}' = \mathfrak{Y}$). It is easy to see that the process will always stop. Moreover, one can check that the configurations that are stable under this refinement process are precisely the coherent configurations. Therefore, the Weisfeiler-Leman refinement process

takes any configuration and refines it to a coherent configuration.

Clearly, the result of a (non-trivial) individualization and the Weisfeiler-Leman refinement is a (non-homogeneous) fission of the original configuration.

Importantly, the Weisfeiler-Leman refinement is *canonical* in the following sense. Let \mathfrak{X} , \mathfrak{Y} be configurations and let \mathfrak{X}^* , \mathfrak{Y}^* be the corresponding outputs of the Weisfeiler-Leman refinement simultaneously applied to \mathfrak{X} and \mathfrak{Y} . Then the sets of isomorphisms for \mathfrak{X} , \mathfrak{Y} and for \mathfrak{X}^* , \mathfrak{Y}^* are the same

$$\operatorname{Iso}(\mathfrak{X},\mathfrak{Y}) = \operatorname{Iso}(\mathfrak{X}^*,\mathfrak{Y}^*) \tag{1.3}$$

1.3.2 Babai's "Split-or-Johnson" Lemma. Robustness of Johnson schemes

The key combinatorial partitioning tool of the Graph Isomorphism algorithm of Babai [2016a,b], the "Split-or-Johnson" lemma, states that one can either find a specific structure or significantly break the symmetry of a coherent configuration after individualizing a logarithmic number of points and applying the Weisfeiler-Leman refinement.

Theorem 1.3.1 (Babai [2016b], "Split-or-Johnson"). Let $\mathfrak{X} = (\Omega, \mathfrak{c})$ be a primitive coherent configuration of rank ≥ 3 on n vertices and let $2/3 \leq \gamma < 1$ be a threshold parameter. Then by individualizing $O(\log n)$ vertices of \mathfrak{X} and by applying the Weisfeiler-Leman refinement process one can get a coherent configuration $\mathfrak{Y} = (\Omega, \mathfrak{c}_{\mathfrak{Y}})$ that satisfies one of the following.

- 1. No color is assigned by $\mathfrak{c}_{\mathfrak{Y}}$ to $\geq \gamma |\Omega|$ vertices.
- 2. $\mathfrak{c}_{\mathfrak{Y}}$ induces a non-trivial equipartition of the vertex color class of size $\geq \gamma |\Omega|$.
- 3. \mathfrak{Y} contains a homogeneous fission of a Johnson scheme on $\geq \gamma |\Omega|$ vertices as a subconfiguration.

Babai conjectured that for a sufficiently large γ in the latter case \mathfrak{X} is either a Johnson scheme itself, or \mathfrak{X} has a quasipolynomial number of automorphisms. In this thesis we make

a step towards confirming this conjecture. This is also a step in the direction of simplifying the conclusion of the "Split-or-Johnson" lemma.

Theorem 1.3.2 (Main III, Babai and Kivva [2022]). Let \mathfrak{Y}' be a homogeneous coherent configuration of rank ≥ 3 on Ω' . Assume that \mathfrak{Y}' is a fusion of a configuration \mathfrak{X}' . Let $\Omega \subseteq \Omega'$, with $n' \leq (6/5)n$. Suppose that $\mathfrak{X} = \mathfrak{X}'[\Omega]$ is the Johnson scheme $\mathfrak{J}(s,d)$ with $s \geq 250d^4$. Then \mathfrak{Y}' is a Johnson scheme itself, of the same rank as \mathfrak{X} .

We present the proof of this Theorem in Section 11.4.2.

1.3.3 Robustness of Hamming and Grassmann schemes

Theorem 1.3.2 can also be seen as an answer to a special case of the following question.

Question 1.3.3. Let $\alpha \geq 0$ and $\Omega \subseteq \Omega'$ be finite sets, such that $|\Omega'| \leq (1+\alpha)|\Omega|$. Assume that $\mathfrak{X}' = (\Omega', \mathfrak{c}')$ and $\mathfrak{X} = (\Omega, \mathfrak{c})$ are homogeneous coherent configurations. Suppose that \mathfrak{X} is "nicely embedded" in \mathfrak{X}' and, moreover, \mathfrak{X} belongs to some class of configurations \mathcal{A} . For which α and \mathcal{A} can we deduce that \mathfrak{X}' also belongs to \mathcal{A} ?

In Chapters 10 and 11 we study this question in the following interpretations of "nicely embedded" for various properties \mathcal{A} .

- (A) \mathfrak{X} is a subconfiguration of \mathfrak{X}' .
- (B) \mathfrak{X} is a subconfiguration of a fission of \mathfrak{X}' .

In particular, we show that analogs of Theorem 1.3.2 hold for Hamming and Grassmann schemes, another two families of schemes that are of interest to several areas of mathematics and theoretical computer science.

Theorem 1.3.4. Let \mathfrak{Y}' be a homogeneous coherent configuration of rank ≥ 3 on Ω' . Assume that \mathfrak{Y}' is a fusion of a configuration \mathfrak{X}' . Let $\Omega \subseteq \Omega'$, with $|\Omega'| \leq (6/5)|\Omega|$. Suppose that

 $\mathfrak{X} = \mathfrak{X}'[\Omega]$ is the Hamming scheme $\mathfrak{H}(d,s)$ with $s \geq 200d^4 \ln(d)$. Then \mathfrak{Y}' is a Hamming scheme, of the same rank as \mathfrak{X} .

Theorem 1.3.5. Let \mathfrak{Y}' be a homogeneous coherent configuration of rank ≥ 4 on Ω' . Assume that \mathfrak{Y}' is a fusion of a configuration \mathfrak{X}' . Let $\Omega \subseteq \Omega'$, with $|\Omega'| \leq (5/4)|\Omega|$. Suppose that $\mathfrak{X} = \mathfrak{X}'[\Omega]$ is the Grassmann scheme $\mathfrak{J}_q(s,d)$ with $s \geq 6d + 5$. Then \mathfrak{Y}' is a Grassmann scheme, of the same rank as \mathfrak{X} , and for the same prime power q.

For Question 1.3.3 in interpretation (A) we prove the following.

Theorem 1.3.6. Let $\mathfrak{X}' = (\Omega', \mathfrak{c}')$ be a homogeneous coherent configuration. Let $\Omega \subseteq \Omega'$ with $|\Omega'| < (3/2)|\Omega|$. Assume that $\mathfrak{X} = \mathfrak{X}'[\Omega]$ is

- (Babai and Kivva [2022]) the Johnson scheme $\mathfrak{J}(d,s)$ with $d \ge 2$, $s \ge 288d^2 + d$; or
- the Hamming scheme $\mathfrak{H}(d,s)$ with $d \geq 2$, $s \geq 200d^4 \ln d$; or
- the Grassmann scheme $\mathfrak{J}_q(s,d)$ with $d \geq 3$ and $s \geq 3d + 7$.

Then \mathfrak{X}' is a Johnson scheme, or a Hamming scheme, or a Grassmann scheme, respectively.

These three theorems are proved in Sections 11.4.3, 11.4.4, and 10.4-10.6.

1.3.4 Group theory view on Question 1.3.3: Galois correspondence

Question 1.3.3 has been studied in the following version of "nicely embedded".

(C) $\Omega = \Omega'$ and \mathfrak{X} is a fission of \mathfrak{X}' .

For this interpretation of "nicely embedded", the question takes the following form.

Question 1.3.7. Assume that $\mathfrak{X}' = (\Omega, \mathfrak{c}')$ and $\mathfrak{X} = (\Omega, \mathfrak{c})$ are homogeneous coherent configurations and \mathfrak{X} is a fission of \mathfrak{X}' . Suppose that \mathfrak{X} belongs to some class of configurations \mathcal{A} . For which \mathcal{A} can we deduce that \mathfrak{X}' also belongs to \mathcal{A} ?

For a finite permutation group $G \leq \text{Sym}(\Omega)$ let $\mathfrak{X}(G)$ be the corresponding Schurian configuration. Note that several groups may define the same Schurian configuration $\mathfrak{X}(G)$. Such groups are called 2-equivalent. The 2-closure of the group G is defined as $\text{Aut}(\mathfrak{X}(G))$, which is the maximal element of the 2-equivalence class of G. The group is called 2-closed if it coincides with its 2-closure.

It is easy to see that if $G \leq G' \leq \operatorname{Sym}(\Omega)$, then $\mathfrak{X}(G)$ is a fission of $\mathfrak{X}(G')$. And vice versa, if \mathfrak{X} is a fission of \mathfrak{X}' , then $\operatorname{Aut}(\mathfrak{X}) \leq \operatorname{Aut}(\mathfrak{X}')$. Recall, that for configurations \mathfrak{X} and \mathfrak{X}' on Ω , we define a partial order by writing $\mathfrak{X} \preceq \mathfrak{X}'$, if \mathfrak{X} is a fission of \mathfrak{X}' . One can check that there is a *Galois correspondence* between the coherent configurations on Ω with the \preceq relation and the 2-closed permutation groups on Ω with the subgroup relation.

In view of this Galois correspondence, results on the fission/fusion of coherent configurations (Question 1.3.3 in interpretation (C)) can be translated into results on the subgroups/supergroups of 2-closed permutation groups.

Recall that $S_t^{(d)} \leq \text{Sym}\left(\binom{[t]}{d}\right)$ is the permutation group defined by the induced action of S_t on *d*-element subsets of [t]. Kaluzhnin and Klin [1972] showed that the Johnson group is a maximal 2-closed subgroup of the symmetric group $\text{Sym}\left(\binom{[t]}{d}\right)$ when $t \geq c(d)$ for a sufficiently large c(d). They proved this by showing that the corresponding Johnson scheme has no nontrivial fusion. In his PhD thesis, Klin [1974] showed that one can take $c(d) = O(d^4)$. Later, Muzychuk [1992a] improved bound to c(d) = 3d + 4 and Uchida [1992] made another slight improvement to $c(d) = 2d + \sqrt{(d - 7/2)^2 + 6} + 3/2$.

Our Theorem 1.3.2 generalizes Kaluzhnin-Klin's theorem.

Similarly, Muzychuk [1992b] proved that the Hamming scheme $\mathfrak{H}(d, s)$ with s > 4 does not admit a non-trivial fusion that is a coherent configuration, and he classified the fusion schemes for s = 4. The case of s = 2 was studied in Muzychuk [1995]. Our Theorem 1.3.4 is as a generalization of Muzychuk [1992b] for $s \ge 200d^4 \ln(d)$.

1.4 Spectral gap and classifications of distance-regular graphs

In order to prove Theorems 1.2.6, 1.2.8 and 1.3.6 which we discussed in Sections 1.2 and 1.3.3, we study spectral and combinatorial properties of distance-regular graphs and coherent configurations. Along the way, we prove several results for distance-regular graphs which fit into several other well-studied frameworks. In particular, we study the spectral gap of distance-regular graphs, the parameter that is closely related to the expansion properties of the graph, and which plays an important role in various applications in combinatorics and theoretical computer science. Additionally, we provide new characterizations of Johnson and Hamming graphs in terms of their smallest eigenvalue and spectral gap. These characterizations can be seen as a contribution to the program that aims to classify sufficiently regular graphs based on their smallest eigenvalue (see, e.g., Hoffman [1970b, 1977], Seidel [1968], Neumaier [1979], Cameron et al. [1991], Bang and Koolen [2014]).

1.4.1 Spectral gap of distance-regular graphs

We say that a k-regular graph is a spectral η -expander for $\eta > 0$, if every non-principal eigenvalue ξ_i of its adjacency matrix satisfies $|\xi_i| \leq k(1 - \eta)$. We say that a graph on nvertices has $(1 - \varepsilon)$ -dominant distance t, if among the $\binom{n}{2}$ pairs of distinct vertices at least $(1 - \varepsilon)\binom{n}{2}$ are at distance t.

In our main result on spectral expansion we show that distance-regular graphs of bounded diameter are spectral expanders if they have $(1 - \varepsilon)$ -dominant distance for sufficiently small $\varepsilon > 0$, depending only on the diameter. This result is one of the key components in the proof of Theorem 1.2.6.

Theorem 1.4.1. For every $d \ge 2$ there exist $\epsilon = \epsilon(d) > 0$ and $\eta = \eta(d) > 0$ such that the following holds. If a distance-regular graph X of diameter d has a $(1-\epsilon)$ -dominant distance, then X is a spectral η -expander.

The key ingredient in the proof of Theorem 1.4.1 is the following new inequality on the intersection numbers of the distance-regular graphs. Essentially, this inequality claims that, if for some j, b_j is large (and therefore, by monotonicity, so are b_i for $i \leq j$) and c_{j+1} is small, then b_{j+1} and c_{j+2} cannot be small simultaneously. In particular, if c_d is sufficiently small, then this inequality shows that b_i do not decrease too fast.

Theorem 1.4.2 (Growth-induced tradeoff). Let X be a distance-regular graph of diameter $d \ge 2$. Let $0 \le j \le d-2$. Assume $b_j > c_{j+1}$ and let $C = b_j/c_{j+1}$. Then for every $1 \le s \le j+1$ we have

$$b_{j+1}\left(\sum_{t=1}^{s}\frac{1}{b_{t-1}} + \sum_{t=1}^{j+2-s}\frac{1}{b_{t-1}}\right) + c_{j+2}\sum_{t=1}^{j+1}\frac{1}{b_{t-1}} \ge 1 - \frac{4}{C-1}.$$
 (1.4)

We prove this inequality in Section 7.2.

In a distance-regular graph, denote by λ and μ the number of common neighbours of a pair of adjacent vertices, and a pair of vertices at distance 2, respectively. We mention, that a result of Terwilliger [1986], as strengthened in [Brouwer et al., 1989, Theorem 4.3.3], shows that every non-principal eigenvalue of a k-regular distance-regular graph X has absolute value at most $k - \lambda$ if $\mu > 1$ and X is not the icosahedron. This result assures that X is a spectral η -expander, if $\lambda \geq \eta k$. We note that while both our result and Terwilliger's result provide simple sufficient combinatorial conditions for being spectral expanders, they are incomparable. In fact, our primary motivation for a spectral gap bound is an application of Lemma 4.5.11, where Terwilliger's gap is not sufficient.

Additionally, we note that in Theorem 1.4.1 we do not exclude the elusive case $\mu = 1$, for which almost no classification results are known, and which is known to be a difficult case in various circumstances. A remarkable example is the Bannai-Ito conjecture, where the case $\mu = 1$ was the only obstacle for 30 years, and was resolved only recently in the breakthrough paper by Bang et al. [2015].

Combining Theorem 1.4.1 with the Metsch characterization of geometric graphs (The-

orem 3.1.3), and Babai's Spectral tool for motion lower bounds (Theorem 4.5.11), in Theorem 8.1.7 we reduce Theorem 1.2.6 to the case of geometric graphs. By exploiting rich structure of geometric graphs, we show that the only such graphs with sublinear motion are Johnson and Hamming graphs. This step relies on the new characterizations of these families of graphs that we discuss below.

1.4.2 New characterizations of Johnson and Hamming graphs

A result of Terwilliger [1986] (see [Brouwer et al., 1989, Theorem 4.4.3]) implies that the icosahedron is the only distance-regular graph, for which the second largest eigenvalue θ_1 (of the adjacency matrix) satisfies $\theta_1 > b_1 - 1$ and a pair of vertices at distance 2 has $\mu \ge 2$ common neighbors. Another classical result gives the classification of distance-regular graphs with $\mu \ge 2$ and $\theta_1 = b_1 - 1$.

Theorem 1.4.3 ([Brouwer et al., 1989, Theorem 4.4.11]). Let X be a distance-regular graph of diameter $d \ge 3$ with second largest eigenvalue $\theta_1 = b_1 - 1$. Assume $\mu \ge 2$. Then one of the following holds:

- 1. $\mu = 2$ and X is a Hamming graph, a Doob graph, or a locally Petersen graph (and all such graphs are known).
- 2. $\mu = 4$ and X is a Johnson graph.
- 3. $\mu = 6$ and X is a half cube.
- 4. $\mu = 10$ and X is a Gosset graph $E_7(1)$.

We consider the case $\theta_1 \geq (1 - \varepsilon)b_1$ for a sufficiently small $\varepsilon > 0$. The relaxation of the assumption on the second largest eigenvalue comes at the cost of requiring additional structural constraints. Our main structural assumption is that X is a geometric distanceregular graph, meaning that there exists a collection of Delsarte cliques (see Sec. 3.1) C such that every edge of X belongs to a unique clique in C. Additional technical structural assumptions depend on whether the neighborhood graphs of X are connected. We note that for a geometric distance-regular graph X either the neighborhood graph X(v) is connected for every vertex v, or X(v) is disconnected for every vertex v (see Lemma 3.2.4). We give the following characterizations.

Theorem 1.4.4 (Main IV). There exists an absolute constant $\varepsilon^* > 0.0065$ such that the following is true. Let X be a geometric distance-regular graph of diameter $d \ge 2$ with smallest eigenvalue -m. Suppose that $\mu \ge 2$ and $\theta_1 + 1 > (1 - \varepsilon^*)b_1$. Moreover, assume that the vertex degree satisfies $k \ge \max(m^3, 29)$ and the neighborhood graph X(v) is connected for some vertex v of X.

Then X is a Johnson graph J(s, d) with s = (k/d) + d.

Theorem 1.4.5 (Main V). Let X be a geometric distance-regular graph of diameter $d \ge 2$ with smallest eigenvalue -m. Consider an arbitrary $0 < \varepsilon < 1/(6m^4d)$. Suppose that $\mu \ge 2$ and $\theta_1 \ge (1 - \varepsilon)b_1$. Moreover, assume $c_t \le \varepsilon k$ and $b_t \le \varepsilon k$ for some $t \le d$, and the neighborhood graph X(v) is disconnected for some vertex v of X.

Then X is a Hamming graph H(d, s) with s = 1 + k/d.

Remark 1.4.6. If $s > 6d^5 + 1$, then the Hamming graph H(d, s) satisfies the assumptions of this theorem with $1/(s-1) \le \varepsilon < 1/(6d^5)$ and t = d.

We present the proof of these theorems in Sections 6.2 and 6.3. These characterizations will be used in Section 8.1 to prove Theorem 1.2.6.

The assumption that a distance-regular graph is geometric excludes only finitely many graphs with $\mu \geq 2$, if the smallest eigenvalue of the graph is assumed to be bounded, as proved by Koolen and Bang [2010].

Theorem 1.4.7 (Koolen and Bang [2010]). Fix an integer $m \ge 2$. There are only finitely many non-geometric distance-regular graphs of diameter ≥ 3 with $\mu \ge 2$ and smallest eigenvalue at least -m. However, in the context of Theorem 1.2.6 we do not have a bound on the smallest eigenvalue in the non-geometric case, so we do not use the above theorem in the proof.

1.4.3 A characterization of Hamming schemes by smallest eigenvalue

A number of classification results is known under the assumption of bounded smallest eigenvalue.

For strongly regular graphs, Neumaier [1979] showed that if the smallest eigenvalue is -m (for $m \ge 2$), then it is a Latin square graph $LS_m(n)$, a Steiner graph $S_m(n)$, a complete multipartite graph or one of finitely many other graphs. A classification of the strongly regular graphs with smallest eigenvalue -2 was known earlier (Seidel [1968]). Moreover, Cameron et al. [1991] gave a complete classification of all graphs with smallest eigenvalue -2. They proved that all but finitely many of such graphs have rich geometric structure (they are generalized line graphs).

Koolen and Bang [2010] proved that all but finitely many distance-regular graphs with smallest eigenvalue -m and $\mu \ge 2$ are geometric. For geometric distance-regular graphs with smallest eigenvalue ≥ -3 and $\mu \ge 2$ Bang [2013] and Bang and Koolen [2014] gave a complete classification. Moreover, they conjectured [Koolen and Bang, 2010, Conjecture 7.4] that for every integer m all but finitely many geometric distance-regular graphs with smallest eigenvalue -m and $\mu \ge 2$ are known.

Conjecture 1.4.8 (Koolen and Bang [2010]). For a fixed integer $m \ge 2$, every geometric distance-regular graph with smallest eigenvalue -m, diameter ≥ 3 and $\mu \ge 2$ is either a Johnson graph, or a Hamming graph, or a Grassmann graph, or a bilinear forms graph, or the number of vertices is bounded above by a function of m.

In this thesis we show that distance-regular graphs of diameter d with smallest eigenvalue -d, $\mu \leq 3$, an induced quadrangle, and sufficiently large degree k are Hamming graphs.

Theorem 1.4.9 (Main VI). Let X be a distance-regular graph of diameter $d \ge 2$ with smallest eigenvalue -d. Suppose that X contains an induced quadrangle, $\mu \le 3$, and $k \ge$ $(100d^3 \ln d) \cdot c_d$. Then X is the Hamming graph H(d, k/d + 1).

The proof of this theorem is discussed in Section 5.2. This characterization also plays a crucial role in our proof of the robustness under extension for Hamming schemes (Theorem 1.3.6, see Section 10.5).

1.5 Acknowledgement of collaborations

Some of the results of this thesis originally appeared in joint papers with László Babai.

In particular, Theorem 1.3.2 and most of the results of Chapters 10 and 11 are a result of joint work by Babai and Kivva [2022]. Only the results on Hamming and Grassmann schemes from these chapters are not a part of this work by Babai and Kivva [2022].

Additionally, the discussion in Section 4.4 is a part of Babai and Kivva [2020].

Most of other original results of this thesis appeared in Kivva [2021a,b,c, 2022].

More precisely, Theorems 1.4.1 and the results of Chapter 7, Section 8.1.3 and 8.4 appeared in Kivva [2021b]. Theorems 1.4.4, 1.4.5 and 1.2.6 and the results of Chapter 6, Section 8.1 and 8.2 first appeared in Kivva [2021c]. The results of Chapter 9 and Theorem 1.2.8 were proved in Kivva [2021a]. Finally, Theorem 1.4.9 and the results of Chapters 10 and 11 related to Hamming and Grassmann schemes are from Kivva [2022].

1.6 Organization of the thesis

We now outline the structure of this thesis. In Chapter 2 we give definitions and discuss basic properties of graphs, groups, coherent configurations and distance-regular graphs. In Chapter 3 we outline preliminaries on geometric distance-regular graphs, a class of a great interest to our analysis. In Chapter 4 we discuss the classification of large primitive groups by Cameron [1981] and the classification of primitive group with sublinear minimal degree by Liebeck and Saxl [1991]. Additionally, in this chapter, we outline the combinatorial and spectral tools for bounding the order and the minimal degree of primitive permutation groups developed by Babai.

In Chapters 5 and 6 we prove our characterizations of Johnson and Hamming graphs, which are used in the proof of Theorem 1.2.6. In this chapter, we also briefly discuss how these results are related to the study of regular graphs with bounded eigenvalue and representation theory of distance-regular graphs.

We prove Theorem 1.4.1 in Chapter 7.

We study motion of distance-regular graphs in Chapter 8 and of primitive coherent configurations of rank-4 in Chapter 9.

Finally, we present our results on robustness of Johnson, Hamming and Grassmann schemes in Chapters 10 and 11.

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