# Computer aided investigation of total graph coherent configurations for two infinite families of classical strongly regular graphs

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## Summary

In this paper we introduce the notion of total graph coherent configuration, and use computer tools to investigate it for two classes of strongly regular graphs – triangular graphs $T(n)$ and lattice square graphs $L_2(n)$. For $T(n)$, we show that its total graph coherent configuration has exceptional mergings only in the cases $n = 5$ and $n = 7$.

## 1 Introduction

The notion of a total graph coherent configuration was introduced and is used in [KliZ], where an imprimitive rank 5 association scheme on 40 points was constructed as a merging of relations in the total graph configuration of the triangular graph $T(5)$.

In this paper we investigate systematically total graph coherent configurations of two infinite series of classical strongly regular graphs.

Section 2 contains all preliminaries which make this presentation mostly self-contained. In Section 3 we consider triangular graphs $T(n)$ and show that in corresponding total graph coherent configuration $\mathcal{T}(n)$ for every $n \geq 6$ there are two merging association schemes with two and three classes. Besides this there are sporadic mergings for the cases $n = 5, 7$. Using a computer we prove that these mergings expire all possible merging association schemes in $\mathcal{T}(n)$. We also show that $\mathcal{T}(n)$ coincides for all $n > 4$ with the Schurian coherent configuration defined by the automorphism group of the total graph of $T(n)$ (this group is actually $S_n$, in action on the edges and paths of length 2 of $K_n$). In Section 4, similar results are presented for the total graph coherent configuration defined by the lattice square graphs $L_2(n)$.

Our results provide an example of successful amalgamation of essential computer algebra experimentation with a subsequent theoretical analysis and generalization. An important feature of presented approach is that the structure constants for both series of coherent configurations appear as polynomials in variable $n$. In Section 5 we present a detailed outline of the used algorithm for the search of mergings which was implemented in GAP.

Finally, in Section 6 we discuss further possibilities for the investigation of the introduced class of coherent configurations. Those include relations to the famous graph isomorphism problem and potential applications of Gröbner bases.

## 2 Preliminaries

### 2.1 Coherent configurations and association schemes

#### 2.1.1 Axioms

Let $X = [1, n]$, $\mathfrak{R} = \{R_1, \ldots, R_r\}$ a collection of binary relations on $X$ (subsets of $X^2$) such that:

CC1 $R_i \cap R_j = \emptyset$ for $1 \leq i \neq j \leq r$;

CC2 $\bigcup_{i=1}^{r} R_i = X^2$;

CC3 $\forall i \in [1, r] \exists i' \in [1, r] R_i^t = R_{i'}$, where $R_i^t = \{(y, x) | (x, y) \in R_i\}$;

CC4 $\exists I' \subseteq [1, r] \bigcup_{i \in I'} R_i = \Delta$, where $\Delta = \{(x, x) | x \in X\}$;

CC5 $\forall i, j, k \in [1, r] \forall (x, y) \in R_k | \{z \in X | (x, z) \in R_i \wedge (z, y) \in R_j\}| = p_{ij}^k$,

then $\mathfrak{M} = (X, R)$ is called a *coherent configuration*. The relations in $R$ are called *basis relations* of $\mathfrak{M}$. The parameters $p_{ij}^k$ are the *structure constants* of the configuration. The graphs $\Gamma_i = (X, R_i)$ are called *basis graphs* of the coherent configuration.

See [Hig70] for original definitions.

Let $(G, \Omega)$ be a permutation group. $G$ acts naturally on $\Omega^2$ by $(x, y)^g = (x^g, y^g)$. Following H. Wielandt in [Wie69], the orbits of this action, $(G, \Omega^2)$ are called the *2-orbits of* $(G, \Omega)$, denoted by $2 - orb(G, \Omega)$.

For every permutation group $(G, \Omega)$, $(\Omega, 2 - orb(G, \Omega))$ is a coherent configuration. Conversely, if the set of relations of a coherent configuration, $\mathfrak{M}$, coincides with $2 - orb(G, \Omega)$ for a suitable group $G$, then $\mathfrak{M}$ is called a *Schurian* coherent configuration.

A coherent configuration which has $\Delta = \{(x, x) | x \in X\}$ as one of its basis relations is called an *association scheme*. In this case, all basis relations except for $\Delta$ are called *classes*.

A *fusion* configuration (or a *merging*) of a coherent configuration $\mathfrak{M} = (X, R)$ is a coherent configuration $\mathfrak{M}' = (X, S)$ on the same set such that each basis relation $S_i$ of $\mathfrak{M}'$ is a union of basis relations of $\mathfrak{M}$.

Coherent configurations can be alternatively described in matrix language. The matrix $A(R)$ of a relation $R$ on $X$ is a $(0,1)$-matrix $A(R) = (a_{ij})$ of dimension $|X| \times |X|$ such that $a_{ij} = 1$ iff $(i,j) \in R$. If $R = \{R_1, \dots, R_r\}$ are basis relations of a coherent configuration then their adjacency matrices $\{A_i = A(R_i)\}_{i=1}^r$ form a basis of a matrix algebra which is closed under Schur-Hadamard (element wise) product.

This leads to equivalent formulation of axioms of coherent configuration:

Let $W \subseteq \mathbb{C}^{n \times n}$ be a matrix algebra of square matrices of order $n$ over the complex field, such that

- CA1 W as a linear space over $\mathbb{C}$ has some basis, $A_1, A_2, \dots, A_r$, consisting of $(0,1)$-matrices;
- CA2 $\sum_{i=1}^{r} A_i = J_n$, where $J_n$ is the square matrix of order $n$ all entries of which are equal to 1;
- CA3 $\forall i \in [1,r] \exists i' \in [1,r] A_i^t = A_{i'}$;
- CA4 $I \in W$ ($I$ denotes the identity matrix),

then $W$ is called a *coherent algebra* of rank $r$ and order $n$ with the *standard basis* $\mathcal{C} = \{A_1, A_2, \dots, A_r\}$. We write $W =< A_1, \cdots, A_r >$.

The notion corresponding to a fusion scheme in this notation is a *coherent subalgebra*, that is a subalgebra which is also a coherent algebra.

### 2.1.2 Weisfeiler-Leman closure

Using matrix notation, it is easy to see that the intersection of coherent algebras is a coherent algebra, and that each square matrix is contained in some coherent algebra (since $M_n(\mathbb{C})$ is coherent). Therefore, we can define the *coherent closure* of a matrix $A$, denoted $<< A >>$ as the smallest coherent algebra containing this matrix (or in other words, the intersection of all coherent algebras containing it).

An efficient algorithm for computing $<< A >>$ was suggested by Weisfeiler and Leman ([Wei76]) and is frequently called the WL-stabilization of the matrix $A$.

### 2.1.3 Wreath product

If $\mathfrak{M}_1 = (X_1, \{R_0, R_1, \dots, R_r\})$ and $\mathfrak{M}_2 = (X_2, \{S_0, S_1, \dots, S_l\})$ are association schemes ($R_0$ and $S_0$ are the reflexive relations), then the wreath product of $\mathfrak{M}_1$ with $\mathfrak{M}_2$ is defined as $\mathfrak{M}_1 \wr \mathfrak{M}_2 = (Y = X_1 \times X_2, \{T_0, T_1, \dots, T_{r+l}\})$ where $T_0$ is the identity relation on $Y$, $T_i = \{((a,b),(c,d)) | (a,c) \in R_i\}$ for all $1 \le i \le r$, and $T_{r+i} = \{((a,b),(a,c)) | (b,c) \in S_i\}$ for all $1 \le i \le l$.

The wreath product of association schemes of ranks $r$ and $l$ is an association scheme of rank $r + l - 1$.

### 2.2 Total Configuration

Let $\Gamma = (V, E)$ be a graph. The *total graph* $T(\Gamma)$ is the graph with the vertex set $V \cup E$, two such vertices in $T(\Gamma)$ are adjacent if and only if they are adjacent or incident in $\Gamma$ (here edges of $\Gamma$ are incident if they have a joint vertex).

A coherent closure of $T(\Gamma)$ will be called a *total coherent configuration* of $\Gamma$.

The *Schurian total coherent configuration* of a graph $\Gamma$ is $(X, 2 - Orb(Aut(T(\Gamma)))$ where X is the set of vertices of $T(\Gamma)$.

The Schurian total configuration has the total configuration as a fusion configuration. Indeed, since an automorphism of $T(\Gamma)$ maps edges of $T(\Gamma)$ to edges, any 2-orbit of $Aut(T(\Gamma))$ either contains edges only, or does not contain edges at all.

### 2.3 Computational tools

#### 2.3.1 COCO

COCO is a set of programs for dealing with coherent configurations. The current version was developed during the years 1990-1992 in Moscow, USSR, mainly by Faradžev and Klin [FarKM94, FarK91].

COCO can be used to construct a coherent configuration $(\Omega, 2-orb(G, \Omega)$, for some prescribed permutation group $(G, \Omega)$, as well as to calculate structure constants, association schemes which are mergings of the coherent configuration, and automorphism groups of those.

COCO was originally written for DOS, and the version currently in use is the UNIX port by A.E. Brouwer, available from Brouwer's home page [Brouwer].

#### 2.3.2 WL-stabilization

Two implementations of the Weisfeiler-Leman stabilization [Wei76] are available, under the name stabil [BCKP97] and stabcol [BabBL96]. The two implementations differ slightly in memory usage and run time, but both are adequate for the coherent configurations used in this article.

#### 2.3.3 GAP

GAP [GAP], [Sch95], an acronym for "Groups, Algorithms and Programming", is a system for computation in discrete abstract algebra. The system is extensible in the sense that it supports easy addition of extensions (packages, in GAP nomenclature), that are written in the GAP programming language which can extend the abilities of the GAP system.

Within GAP framework, COCO-II (a reimplementation of COCO functionality as a GAP package, currently in development by S. Reichard et al) will be used. COCO-II improves on original COCO by adding functionality such as WL-stabilization, as well as using algorithms developed since the release of COCO.

The author modified some COCO-II functions to handle polynomial structure constants, instead of the usual numeric constants, and those functions are used to handle the general case in this paper.

## 3 Total configuration of triangular graph

### 3.1 Definition and basic properties

We are interested in the total coherent configuration $\mathcal{T}(n)$ of the triangular graph $T(n)$ (recall that $T(n)$ is the line graph $L(K_n)$ of the complete graph $K_n$).

In more detail, the total graph $\mathbb{T}(n)$ is the total graph of the triangular graph $T(n)$. The vertices of $\mathbb{T}(n)$ are the edges and the paths of length 2 of $K_n$, and two vertices (of $\mathbb{T}(n)$) are joined if they are both edges of $K_n$ that have a point (of $K_n$) in common, or else they have an edge of $K_n$ in common. $\mathbb{T}(n)$ has $\frac{n(n-1)^2}{2}$ vertices. $\mathcal{T}(n)$ is the coherent closure of $\mathbb{T}(n)$.

To investigate $\mathcal{T}(n)$ we will first consider the Schurian total coherent configuration $\mathcal{S}(n)$, and later show that $\mathcal{T}(n) = \mathcal{S}(n)$.

Let $\Omega$ be the set of vertices of $\mathbb{T}(n)$. In other words,

$$\Omega = \{\{a,b\} | a \neq b \in [1,n]\} \cup \{\{\{a,b\},\{a,c\}\} | a,b,c \in [1,n], a \neq b, a \neq c, b \neq c\}.$$

Let $G$ be the automorphism group of $\mathbb{T}(n)$; it is well known that $G$ is the permutation group $(S_n, \Omega)$ (with the natural action of $S_n$ on $\Omega$) for $n > 4$. Then, $\mathcal{S}(n) = (\Omega, 2 - orb(G))$ is the Schurian total coherent configuration of the triangular graph.

For $n \geq 6$, $\mathcal{S}(n)$ has 2 fibres and 25 relations as follows: (for the sake of brevity, we will list a standard compact description for each relation).

Two reflexive relations:
$R_0 = (\{a,b\},\{a,b\})$,
$R_1 = (\{\{a,b\},\{a,c\}\},\{\{a,b\},\{a,c\}\})$,
Two relations within first fibre:
$R_2 = (\{a,b\},\{a,c\})$ (arcs of the triangular graph),
$R_3 = (\{a,b\},\{c,d\})$ (arcs of its complement),
five relations between first and second fibre:
$R_4 = (\{a,b\},\{\{c,d\},\{c,e\}\})$,

$R_5 = (\{a,b\},\{\{a,c\},\{a,d\}\})$,
$R_6 = (\{a,b\},\{\{c,a\},\{c,d\}\})$,
$R_7 = (\{a,b\},\{\{a,b\},\{a,c\}\})$,
$R_8 = (\{a,b\},\{\{c,a\},\{c,b\}\})$,
and the five inverses $R_9,\ldots,R_{13}$ respectively,
eleven relations within second fibre:
$R_{14} = (\{\{a,b\},\{a,c\}\},\{\{d,e\},\{d,f\}\})$,
$R_{15} = (\{\{a,b\},\{a,c\}\},\{\{a,d\},\{a,e\}\})$,
$R_{16} = (\{\{a,b\},\{a,c\}\},\{\{d,a\},\{d,e\}\})$,
$R_{17} = (\{\{a,b\},\{a,c\}\},\{\{b,d\},\{b,e\}\})$,
$R_{18} = (\{\{a,b\},\{a,c\}\},\{\{d,b\},\{d,e\}\})$,
$R_{19} = (\{\{a,b\},\{a,c\}\},\{\{a,b\},\{a,d\}\})$,
$R_{20} = (\{\{a,b\},\{a,c\}\},\{\{b,a\},\{b,d\}\})$,
$R_{21} = (\{\{a,b\},\{a,c\}\},\{\{d,a\},\{d,b\}\})$,
$R_{22} = (\{\{a,b\},\{a,c\}\},\{\{d,b\},\{d,c\}\})$,
$R_{23} = (\{\{a,b\},\{a,c\}\},\{\{b,c\},\{b,d\}\})$,
$R_{24} = (\{\{a,b\},\{a,c\}\},\{\{b,a\},\{b,c\}\})$.

(Note, that of those, 14, 15, 18, 19, 20, 22 and 24 are symmetric, $(16,17)$ $(21,23)$ are the anti-symmetric pairs.

| Relation | Size | Relation | Size |
|---|---|---|---|
| 0 | $\binom{n}{2}$ | 1 | $3\binom{n}{3}$ |
| 2 | $n(n-1)(n-2)$ | 3 | $\binom{n}{2}\binom{n-2}{2}$ |
| 4 | $\binom{n}{2}(n-2)\binom{n-3}{2}$ | 5 | $\binom{n}{2}2\binom{n-2}{2}$ |
| 6 | $\binom{n}{2}2(n-2)(n-3)$ | 7 | $\binom{n}{2}2(n-2)$ |
| 8 | $\binom{n}{2}(n-2)$ | 14 | $n\binom{n-1}{2}(n-3)\binom{n-4}{2}$ |
| 15 | $n\binom{n-1}{2}\binom{n-3}{2}$ | 16 | $n\binom{n-1}{2}(n-3)(n-4)$ |
| 17 | $n\binom{n-1}{2}2\binom{n-3}{2}$ | 18 | $n\binom{n-1}{2}2(n-3)(n-4)$ |
| 19 | $n\binom{n-1}{2}2(n-3)$ | 20 | $n\binom{n-1}{2}2(n-3)$ |
| 21 | $n\binom{n-1}{2}2(n-3)$ | 22 | $n\binom{n-1}{2}(n-3)$ |
| 23 | $n\binom{n-1}{2}2(n-3)$ | 24 | $n\binom{n-1}{2}2$ |

**Table 1.** Sizes of basis relations of $\mathcal{S}(n)$

The set of edges of the total graph of the triangular graph is the union

$$R_2 \cup R_7 \cup R_{12} \cup R_{19} \cup R_{20} \cup R_{24}.$$

### 3.2 Structure constants of $\mathcal{S}(n)$

**Proposition 1** *The structure constants of $\mathcal{S}(n)$ are functions of $n$. For $n \geq 9$, each such function is a polynomial function in $n$ of degree at most 3.*

*Proof.* To calculate a structure constant $p_{i,j}^k$, we take the general representative pair, $(X,Y)$, of $R_k$, and try to find a general vertex $Z$ such that

$(X,Z) \in R_i$ and $(Z,Y) \in R_j$. The selection of $(X,Y)$ partitions the points $[1,n]$ into at most 6 parts of constant size (not dependent on n, but dependent on $X,Y$), and one part of size $n-k$ where $k$ is again dependent on $X,Y$ but not on $n$. So, the number of ways of selecting $Z$ is a product of two or three of the sizes of parts, or sizes of parts minus one, or sizes of parts minus 2 (or maybe half this product, in case a set of two points needs to be selected), and therefore is a polynomial of degree at most 3 in $n$.

Examples:

If we want to calculate $p^{15}_{10,5}$:

$(\{\{a,b\},\{a,c\}\},\{\{a,d\},\{a,e\}\})$ partitions the set $[1,n]$ to parts $\{a\}$, $\{b,c\}$, $\{d,e\}$, and the rest, of size $n-5$. A vertex $\{x,y\}$ such that $(\{\{a,b\},\{a,c\}\},\{x,y\})$ is in $R_{10}$ and $(\{x,y\},\{\{a,d\},\{a,e\}\})$ is in $R_5$ must satisfy $x \in \{a\}$, $y \notin \{a,b,c\}$, $x \in \{a\}$, $y \notin \{a,d,e\}$. We have one way of selecting $x$ and $n-5$ ways of selecting $y$, so $p^{15}_{10,5} = n-5$.

If we want to calculate $p^{14}_{14,14}$:

$(\{\{a,b\},\{a,c\}\},\{\{d,e\},\{d,f\}\})$ partitions $[1,n]$ into $\{a\}$, $\{b,c\}$, $\{d\}$, $\{e,f\}$, and we need to find $\{\{x,y\},\{x,z\}\}$ such that $x,y,z \notin \{a,b,c,d,e,f\}$, so we have $n-6$ ways to select $x$ and $\frac{(n-7)(n-8)}{2}$ ways to select $y$ and $z$, so $p^{14}_{14,14} = \frac{(n-6)(n-7)(n-8)}{2}$.

This last example shows why we need to assume $n \geq 9$ for the general argument. This is the case that requires the maximal number of points from the original graph $K_n$.

Now we can use a computer to calculate the actual polynomials: Using COCO, we found numerical values for all structure constants in the cases $n = 9, 10, 11, 12$. Then for each triplet $i,j,k$ we used Lagrange interpolation in GAP to find the polynomial $p^k_{i,j}(n)$.

### 3.3 Mergings of $\mathcal{S}(n)$

Looking at mergings of $\mathcal{S}(n)$ (for $n \geq 6$) resulting in association schemes, we see that in the general case there are only two mergings:

A strongly regular graph, $\Gamma$, with parameters $(\frac{n(n-1)^2}{2}, n-2, n-3, 0)$. This SRG is union of relations $R_8 \cup R_{13} \cup R_{22}$. This graph can be defined on the vertices of $\mathbb{T}(n)$, denoted by $\{a,b\}$ and $(\{a,b\},c)$ (the latter standing for $\{\{a,c\},\{b,c\}\}$), as follows: an edge between two vertices is if they share the same two-set. Since $\mu = 0$, this graph is isomorphic to $\frac{n(n-1)}{2}$ copies of $K_{n-1}$.

A rank 4 association scheme, whose classes are the unions of relations:

$R_0 \cup R_1$;

$R_8 \cup R_{13} \cup R_{22}$;

$R_2 \cup R_6 \cup R_7 \cup R_{11} \cup R_{12} \cup R_{18} \cup R_{19} \cup R_{21} \cup R_{23} \cup R_{24}$;

$R_3 \cup R_4 \cup R_5 \cup R_9 \cup R_{10} \cup R_{14} \cup R_{15} \cup R_{16} \cup R_{17} \cup R_{20}$.

When using the above notation ($\{a,b\}$ and $(\{a,b\},c)$) for the set of vertices of $\mathbb{T}(n)$, the relations of this merging association scheme can be defined by the number of points their two-sets share.

With this observation we recognize that the rank 4 scheme is wreath product $\mathfrak{M} \wr K_{n-1}$, where $\mathfrak{M}$ is the rank 3 association scheme with basis graphs $\Delta$, $T(n)$, and $\overline{T(n)}$.

The only exception is for $n = 7$ which has another SRG as a merging of the relations: $R_3 \cup R_4 \cup R_8 \cup R_9 \cup R_{13} \cup R_{15} \cup R_{18} \cup R_{20}$. This SRG has parameters $(126, 45, 12, 18)$, and will be discussed in subsequent publication [KliZJ].

For $n = 5$, relation $R_{14}$ is actually empty, since it requires 6 different points of $K_n$. So $\mathcal{S}(5)$ is rank 24 coherent configuration. This configuration has 9 merging association schemes listed in Table 2. Some of the mergings are discussed in [KliZ], [KliZJ].

| rank | mergings | $\|aut\|$ | SRG parameters |
|---|---|---|---|
| 5 | $(3, 4, 5, 9, 10, 15, 16, 17, 20)$<br>$(8, 13, 22)$<br>$(2, 7, 12, 18, 19, 24)$<br>$(6, 11, 21, 23)$ | 1920 | |
| 5 | $(3, 4, 9, 15, 20)$<br>$(8, 13, 22)$<br>$(5, 10, 16, 17)$<br>$(2, 6, 7, 11, 12, 18, 19, 21, 23, 24)$ | 7680 | |
| 5 | $(3, 7, 8, 12, 13, 15, 16, 17, 18)$<br>$(4, 9, 24)$<br>$(2, 5, 10, 19, 20, 22)$<br>$(6, 11, 21, 23)$ | 1920 | |
| 5 | $(3, 8, 13, 15, 18)$<br>$(4, 9, 24)$<br>$(2, 5, 6, 10, 11, 19, 20, 21, 22, 23)$<br>$(7, 12, 16, 17)$ | 7680 | |
| 4 | $(3, 4, 5, 9, 10, 15, 16, 17, 20)$<br>$(8, 13, 22)$<br>$(2, 6, 7, 11, 12, 18, 19, 21, 23, 24)$ | $2^{33}3^{11}5$ | |
| 4 | $(3, 7, 8, 12, 13, 15, 16, 17, 18)$<br>$(4, 9, 24)$<br>$(2, 5, 6, 10, 11, 19, 20, 21, 22, 23)$ | $2^{33}3^{11}5$ | |
| 3 | $(2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 15, 16,$<br>$17, 18, 19, 20, 21, 23, 24)$<br>$(8, 13, 22)$ | $2^{38}3^{14}5^27$ | $(40, 3, 2, 0)$ |
| 3 | $(2, 3, 4, 5, 7, 8, 9, 10, 12, 13, 15, 16,$<br>$17, 18, 19, 20, 22, 24)$<br>$(6, 11, 21, 23)$ | 51840 | $(40, 12, 2, 4)$ |
| 3 | $(2, 3, 5, 6, 7, 8, 10, 11, 12, 13, 15, 16,$<br>$17, 18, 19, 20, 21, 22, 23)$<br>$(4, 9, 24)$ | $2^{38}3^{14}5^27$ | $(40, 3, 2, 0)$ |

(All mergings also merge reflexive relations, $R_0$ and $R_1$)

**Table 2.** Mergings of $\mathcal{S}(5)$

### 3.4 $\mathcal{S}(n)$ and $\mathcal{T}(n)$

**Proposition 2** $\mathcal{S}(n) = \mathcal{T}(n)$

*Proof.* First we recall that the total graph $\mathbb{T}(n)$ is a union of the relations $R_2 \cup R_7 \cup R_{12} \cup R_{19} \cup R_{20} \cup R_{24}$, so $\mathcal{T}(n)$ is a fusion configuration of $\mathcal{S}(n)$. It is enough to show that no proper fusion configuration of $\mathcal{S}(n)$ contains $\mathbb{T}(n)$.

For $4 < n < 9$ we check by a computer implementation of the Weisfeiler-Leman closure algorithm that the closure of the total graph is indeed the configuration $\mathcal{S}(n)$ (without empty relation $R_{14}$ in the case $n = 5$). By using COCO, we find that for $n \geq 6$ there are two fusion association schemes of ranks 3 and 4, except for $n = 7$ where there is another scheme of rank 3.

For $n \geq 9$, we confirm by computer search that those two mergings always appear, no other mergings appear for all $n$, and there are no sporadic mergings other then those described in 3.3.

This proves that $\mathcal{S}(n) = \mathcal{T}(n)$, since $\mathcal{T}(n)$ is a merging of $\mathcal{S}(n)$, but the mergings we found do not admit $\mathbb{T}(n)$ as a union of relations.

## 4 Total configuration of $L_2(n)$

### 4.1 Definition and basic properties.

The lattice square graph, $L_2(n)$, is a graph with $n^2$ vertices, usually the vertex set is denoted by $\{1, 2, \ldots, n\}^2$, with $(a, b)$ adjacent to $(c, d)$ if $a = c$ or $b = d$. It is usefull to regard the vertices as points in the $n \times n$-grid. Two vertices are adjacent if and only if they are in the same row or the same column. For our purposes it is also useful to see this graph as the line graph of the complete bipartite graph $K_{n,n}$.

$L_2(n)$ is a regular graph of valency $2(n-1)$, so it has $n^2(n-1)$ edges. The total graph $T(L_2(n))$ has $n^2 + n^2(n-1) = n^3$ vertices.

Let us denote vertices of $L_2(n)$ by $(a, x)$, where $a, x \in \{1, \ldots, n\}$. The automorphism group $G = Aut(L_2(n))$ of order $2(n!)^2$ is generated by $S_n$ acting on first coordinate, $S_n$ acting on second coordinate, and involution mapping $(a, x)$ to $(x, a)$, denoted by $t$. In other words, $G$ is the exponentiation $S_n \uparrow S_2$, as in [FarKM94].

In this notation, edges of $L_2(n)$ are of the form $\{(a, x), (a, y)\}$ (a pair of vertices in the same row) or $\{(x, a), (y, a)\}$ (a pair of vertices in the same column).

We shall denote total coherent configuration of $L_2(n)$ by $\mathfrak{T}(n)$ and Schurian total configuration of $L_2(n)$ by $\mathfrak{S}(n)$.

In the following listing of representatives of relations of $\mathfrak{S}(n)$, $a, b, c, d$ stand for distinct elements of $[1..n]$, and $x, y, z, w$ stand for distinct elements of $[1..n]$. The sets $\{a, b, c, d\}$ and $\{x, y, z, w\}$ are not necessarily disjoint.

In relations $R_4, \ldots, R_{11}$ the representative of edges appear all as a pair of vertices in the same row. Since the involution $t$ is in the automorphism group, and maps a pair of vertices in the same row to a pair of vertices in the same column, those edges are also represented. For example, $((a,x),\{(a,x),(b,x)\})$ is in $R_4$, since it is the result of action of $t$ on $((x,a),\{(x,a),(x,b)\})$ which is clearly in $R_4$.

In the same manner, when looking at relations $R_{12},\ldots,R_{20}$ (pairs of edges of $L_2(n)$), it does not matter if the first edge is a pair of vertices in the same row or a pair of vertices in the same column, but it does matter whether both edges are of the same kind (row or column) or of different kinds. Relations $R_{12},\ldots,R_{16}$ are of the former type, while relations $R_{17},\ldots,R_{20}$ are of the latter type.

$\mathfrak{S}(n)$ has the following 21 relations (for $n \geq 3$):

Reflexive relations:

$R_0 = ((a,x),(a,x))$
$R_1 = (\{(a,x),(a,y)\},\{(a,x),(a,y)\})$

Relations within first fibre:

$R_2 = ((a,x),(a,y))$
$R_3 = ((a,x),(b,y))$

Relations between first and second fibre:

$R_4 = ((a,x),\{(a,x),(a,y)\})$
$R_5 = ((a,x),\{(b,x),(b,y)\})$
$R_6 = ((a,x),\{(a,y),(a,z)\})$
$R_7 = ((a,x),\{(b,y),(b,z)\})$

Their inverses:

$R_8 = (\{(a,x),(a,y),(a,x)\})$
$R_9 = (\{(b,x),(b,y),(a,x)\})$
$R_{10} = (\{(a,y),(a,z),(a,x)\})$
$R_{11} = (\{(b,y),(b,z),(a,x)\})$

And relations within second fibre:

$R_{12} = (\{(a,x),(a,y)\},\{(a,x),(a,z)\})$
$R_{13} = (\{(a,x),(a,y)\},\{(a,z),(a,w)\})$
$R_{14} = (\{(a,x),(a,y)\},\{(b,x),(b,y)\})$
$R_{15} = (\{(a,x),(a,y)\},\{(b,x),(b,z)\})$
$R_{16} = (\{(a,x),(a,y)\},\{(b,z),(b,w)\})$
$R_{17} = (\{(a,x),(a,y)\},\{(a,x),(b,x)\})$
$R_{18} = (\{(a,x),(a,y)\},\{(a,z),(b,z)\})$
$R_{19} = (\{(a,x),(a,y)\},\{(b,x),(c,x)\})$
$R_{20} = (\{(a,x),(a,y)\},\{(b,z),(c,z)\})$

$R_{18}$ and $R_{19}$ form an anti-symmetric pair. All other relations within second fibre are symmetric.

The total graph $T(L_2(n))$ is the union of the relations: $R_2 \cup R_4 \cup R_8 \cup R_{12} \cup R_{17}$.

| Relation | Size | Relation | Size |
|---|---|---|---|
| 0 | $n^2$ | 1 | $n^2(n-1)$ |
| 2 | $2n^2(n-1)$ | 3 | $n^2(n-1)^2$ |
| 4 | $2n^2(n-1)$ | 5 | $2n^2(n-1)^2$ |
| 6 | $n^2(n-1)(n-2)$ | 7 | $n^2(n-1)^2(n-2)$ |
| 12 | $2n^2(n-1)(n-2)$ | 13 | $\frac{1}{2}n^2(n-1)(n-2)(n-3)$ |
| 14 | $n^2(n-1)^2$ | 15 | $2n^2(n-1)^2(n-2)$ |
| 16 | $\frac{1}{2}n^2(n-1)^2(n-2)(n-3)$ | 17 | $2n^2(n-1)^2$ |
| 18 | $n^2(n-1)^2(n-2)$ | 19 | $n^2(n-1)^2(n-2)$ |
| 20 | $\frac{1}{2}n^2(n-1)^2(n-2)^2$ | | |

**Table 3.** Sizes of basis relations of $\mathfrak{S}(n)$

### 4.2 Structure constants of $\mathfrak{S}(n)$

As in the case of the complete graph in the previous section, when we calculate $p_{ij}^k$ for a given triplet $(i, j, k)$, we actually take an element $(M, N)$ of relation $R_k$, and count the amount of elements $P$ such that $(M, P) \in R_i$ and $(P, N) \in R_j$. $P$ is either a vertex or an edge of $L_2(n)$, so we need to select two or three elements of $[1..n]$. For each element of $[1..n]$ that we need to select, it either needs to be one already used in $M$ or $N$, in which case the number of options is a constant independent of $n$, or not used, in which case the number of options is $n - r$, where $r$ is dependent on $i$, $j$, $k$, but not on $n$. After all selections, we might need to multiply by 2 (if the representative element of $R_i$ is not invariant under the involution $t$), and similarly for $R_j$ an $R_k$. We also need to divide by 2, if $P$ is and edge of $L_2(n)$, since we selected two elements the order of which is irrelevant. Finally, we conclude that $p_{ij}^k$ is a polynomial function in $n$ of degree at most 3.

For finding the minimal $n$ for which this argument will work, we note that the worst case is in calculation of $p_{16,16}^{16}$, where we have pair $(\{(a, x), (a, y)\}, \{(b, z), (b, w)\})$, and need to find an edge of $L_2(n)$ $\{(c, u), (c, v)\}$, such that $u$ is different from $x, y, w, z$, and so is $v$. In conclusion:

**Proposition 3** *The structure constants of $\mathfrak{S}(n)$ are functions of $n$. For $n \geq 6$, each such function is a polynomial function in $n$ of degree at most 3.*

### 4.3 Mergings of $\mathfrak{S}(n)$

$\mathfrak{S}(n)$ admits no association schemes as mergings (for $n \geq 3$).

### 4.4 $\mathfrak{S}(n)$ and $\mathfrak{T}(n)$

**Proposition 4** $\mathfrak{S}(n) = \mathfrak{T}(n)$

*Proof.* First we recall that the total graph $T(L_2(n))$ is a union of the relations $R_2 \cup R_4 \cup R_8 \cup R_{12} \cup R_{17}$. So, $\mathfrak{T}(n)$ is a fusion configuration of $\mathfrak{S}(n)$. It is enough to show that no proper fusion configuration of $\mathcal{S}(n)$ contains $\mathbb{T}(n)$. This is done by computer search.

## 5 Details of computer search

The computer search mentioned in sections 3.4 and 4.4 is based on the notion of good sets, which goes back to [FarKM94]:

If $W =< A_0, \ldots, A_r >$ is a coherent algebra, then we define a good set to be a subset $B \subseteq [0..r]$ such that:

GS1 $M = \sum_{i \in B} A_i$ is a symmetric or an anti-symmetric matrix;

GS2 if $M^2 = \sum_{i=0}^{r} b_i A_i$ then for every $i, j \in B$, $b_i = b_j$;

GS3 $I \circ M = M$ or $I \circ M = 0$ ($\circ$ is Schur-Hadamard product).

With this definition of a good set, we see that for a partition $P = \{P_1, \ldots, P_k\}$ of $[0..r]$ to induce a coherent subalgebra, each $P_i$ must be a good set. This reduces the computational search for subalgebras from a search through all partitions of $[0..r]$, to a search through partitions consisting of good sets only.

This method, originally developed in [FarKM94] for use with a numerical tensor of structure constants, also works for a polynomial tensor. A set that is good by it's polynomial parameters, that is good for all $n \geq 9$, is called *polynomially good set*.

I The graphs $\mathbb{T}(n)$ are constructed for $n = 9, 10, 11, 12$, and for each such $n$, the WL-closure, $\mathcal{T}(n)$ is calculated. We then check that it coincides with $\mathcal{S}(n)$, which is calculated by COCO.

II The structure constants of the four coherent configurations are used to generate the polynomial tensor of structure constants (using Lagrange interpolation).

III Instead of searching for all mergings, we limit our search to specific kinds of mergings:

i Mergings resulting in association schemes: This adds another requirement for a good set: for $B$ to be a good set, the graph with edge set $\bigcup_{i \in B} R_i$ must be regular. This additional requirement leaves 5 good sets and quick search shows that only two mergings (those described in 3.3) appear.

ii Mergings that admit $\mathcal{T}(n)$ as a merging. This means that $Q = \{2, 7, 12, 19, 20, 24\}$ is a union of sets from the partition, or in other words an additional condition for good sets $R$ is that either $R \subseteq Q$ or $R \cap Q = \emptyset$. Since none of the previous two mergings fulfill this condition, we know that such mergings do not result in association schemes.

Since we only have two fibres, this means that the mergings we are looking for also have two fibres. This allows us to partition the relations into cells according to fibres:

$$\{\{0\},\{1\},\{2,3\},\{4,5,6,7,8\},\{9,10,11,12,13\},\{14,\ldots,24\}\}$$

and require a good set to comply with partition, that is, to be a subset of one of the sets in the partition.

Those two conditions leave 48 good sets and a simple search shows that none of the partitions result in a coherent configuration.

IV The previous step is enough to show that there is no merging (except for the two described in 3.3) that appear for every $n \geq 9$. To confirm that no other mergings appear for particular $n > 7$ we use the following principle: When we check if a set $B = \{a_1, \ldots, a_l\}$ is good, we actually calculate the sums $Q_k = \sum_{i,j \in B} p_{i,j}^k$ for each $k \in B$. Clearly, if all these sums are equal, then the set is good. If it is not good, then we have (at least) two elements $i, j \in B$ such that the polynomials $Q_i$ and $Q_j$ differ. If a natural number $n_0$ is a root of the polynomial $Q_i - Q_j$, it means that while the set $B$ is not a good set for all $n$, it might be a good set for $n_0$. In this case we add this $n_0$ to the list of $n$ for which an exceptional merging might appear.

In the case of $\mathcal{S}(n)$, the list of possible exceptions included all the integers in the range [1..22], and a computerized brute force search shows that for no $n$ in the range $7 < n \leq 22$, an exceptional merging appear.

A similar search is performed for the total configurations of the lattice square graphs. In this case there were no mergings resulting in association schemes which appear for all $n$, and the list of possible exceptions is $\{3,4,5,6,7,8,9,10,11,17\}$. A computerized search shows that there is no exceptional merging resulting in an association scheme for any of those values.

## 6 Conclusions

It is easy to check that the total graph of the complete graph $K_n$ with $n$ vertices is isomorphic to the triangular graph $T(n+1)$. This observation by [BehCN68], see also [Har69] was one of the earliest stimuli of interest to this concept.

We again refer to [KliZ] for a detailed discussion of exceptional Schurian association scheme with the automorphism group of order 1920 which appears as a merging of classes in $\mathcal{T}(5)$.

The triangular graph $T(5)$ is a complement of the Petersen graph. Petersen graph may be considered as the smallest Moore graph (see, e.g. [CamvL91]).

This is why we are also investigating the total graph configurations of the complements of the unique Moore graph of valency 7 and of a potential Moore graph of valency 57, see [KliZJ].

It seems as a very attractive task to search for other examples of strongly regular graphs, which have total coherent configuration admitting exceptional mergings. Our results for the graphs $L_2(n)$ provide a small evidence for believing that such examples are quite rare.

We hope that the use of Gröbner bases (cf. [Leo]) may help in computerized investigation of other infinite series of classical strongly regular graphs.

The problem of the description of the 2-orbits of the automorphism group of an arbitrary graph $\Gamma$ is closely related to the graph isomorphism problem, see e.g. [KliRRT99]. In case when for a graph $\Gamma$ its total graph coherent configuration and the Schurian total graph coherent configuration coincide, using WL-closure, we get as a by-product a polynomial-time procedure for the description of $2-orb(Aut(\Gamma))$. At this moment we are not aware of an example where those two coherent configurations are distinct. Certain possibilities for such counterexamples will be discussed in [KliZJ], in particular, in view of the results from [EvdP99] and related publications.

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