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Geometric methods in algebraic graph theory

1 Individual Project's contribution to the CRP

The main areas of research of the AP are algebraic graph theory (AGT) and computer algebra. The techniques exploited in AGT could be considered as a common roof over group theory, linear algebra, geometry, etc. with the goal of enumerating and classifying graphs with diverse properties related to their symmetry. Tradition of the use of geometric methods in AGT goes back to the works of R. C. Bose and J. J. Seidel, both geometers by training. Spirit of Coxeter is of extraordinary significance in AGT, see e.g. [8], the bible of this area.

Two significant lines of an interplay between AGT and geometry are related to incidence geometries and representations of graphs. Partial geometries, as defined in [7], are an ingredient of incidence geometries with geometric strongly regular graphs (SRGs) in the role of the point graphs. The concept of an (Euclidean) representation of a graph, rigorously defined in [8], pp. 87–90 allows to establish an extraordinary proficient impact between techniques of geometry and AGT. The links between spherical designs and SRGs serve as a bright example [3], [2].

From its inception, [5], the goal in AGT is classification of "exceptionally beautiful" graphs, where criteria of beauty are formulated in terms of group theoretical, combinatorial and geometrical regularity. Five classical Platonic solids are nothing else but initial triumph of the coherence between these three sources of the requirements [8]. Just recently it became clear that some infinite series and sporadic examples of nice graphs, discovered in AGT, serve as a source of abstract analogues of a similar coherence in high-dimensional Euclidean spaces, see e.g. [1].

Methods of computer algebra and symbolic computation during last decade proved their efficiency on the edge between geometry and graph theory, see e.g. [13]. To each graph Γ, having an Euclidean representation in $\mathbb{R}^n$ we may attribute groups $Aut(\Gamma)$ and $Iso(\Gamma)$ of its combinatorial and geometrical symmetries (automorphisms and isometries respectively). Clearly $Iso(\Gamma) \leq Aut(\Gamma)$, cf. naive discussion in [11]. The equality of these groups means that the considered representation is in a sense natural. Drawing of a graph Γ is also a kind of its geometrical representation. The fulfillment of the polycirculant conjecture (due to Marušič-Klin), see [9], implies, in particular, that one may find a nice standard drawing of Γ, with the aid of suitable simple rules of the game. A lot of such attractive diagrams are available, e.g. from [17]. One more area of applications is related to discrete geometry, and in particular to the use of oriented matroids [6]. The AP was one of the pioneers to apply this concept [12] for the modeling of stereo-isomers of organic compounds. The use of modern computer technology (see paper R2 by R. Gugich in [13]) opens new promising horizons.

1.1 Aims and Objectives

Part 1. We will hunt for new examples of association schemes of small rank which may be naturally described in geometric terms, in particular via root systems for suitable Coxeter groups.
Part 2. To each vertex-transitive graph Γ one may attribute its *polycirculant* index, that is the smallest value m, such that $Aut(\Gamma)$ contains a semiregular cyclic group with m orbits on vertices. The *circulant* graphs (the ones with the index 1) are the best from the point of view of graph drawings. A possible diversity of such index m will be experimentally investigated.
Part 3. A new concept of a Deza family in Higmanian house was coined in [14]. A geometrical Higmanian house is a suitable incidence geometry. First examples of such objects, on 40 points are completely classified; the one having the highest symmetry stems from a Coxeter group D_5 and is related to [1]. We will arrange a search for new larger examples of such structures.

Primitive SRGs with no triangles are exceptionally rare. Only 7 such graphs are known, all are induced subgraphs of the graph $NL_2(10)$, the unique SRG with the parameters (100,22,0,6), aka the Higman-Sims graph. In fact, the graph $NL_2(10)$ was established by D. Mesner (1956, 1964), (see [15]). It appears also in [1] as an exceptional geometrical representation on 22-dimensional sphere. We will pursue an ambitious lead: to search for new examples of SRGs

with no triangles, relying on [15], new methods from [16] and use of computer algebra packages.
Part 4. Relying on the parameters of partial geometries (K, R, T) as were originally defined by Bose [7], we will select a handful of parameter sets, for which the goal will be or to provide a computer free proof of the completeness of known catalogs, or a solution to the question of existence, or complete classification with the aid of a computer. Geometries on 45, 75, 120, 275 points provide a selection of tasks from realistic to quite ambitious ones.
Part 5. Investigation of fullerenes is one of the greatest achievements in modern mathematical chemistry. Traditional mathematical model of a fullerene is a graph. However (as for each organic compound) stereomodel is also of a great significance. Each fullerene clearly may be regarded as a polytope, which may be embedded to a sphere. It was Seidel who coined a very promising tool (approximation of sphere of strength t) in his paper "The football", [19] pp. 363–371. Moreover, two representations of the classical fullerene on 60 points of strength 9 and 10 respectively were presented in the mentioned text. A careful comparison of these (an other possible representations) with the goal of further investigations provide a promising impetus.

Another attractive lead is related to so-called graph-set analysis, a new mathematical tool in chemical crystallography, which was developed during last two decades, mainly due to efforts of J. Bernstein (Beer Sheva) and his collaborators, see e.g. [4], [10], [18]. The existence of molecular crystals is due to the cumulative effect of small interactions between different molecules with a special significance of hydrogen bonds. Mathematical modelling of such interactions, originally (due to A. I. Kitaigordsky) was fulfilled in naive terms of packing of molecules in a 3D-space. Nowadays a molecule is regarded as a geometrical graph in which each vertex is assigned to a point in a space. A crystal appears as a connected (potentially infinite) graph, in which additional edges (due to the hydrogen bonds) adjoin different molecules. This was started in 1995–2000 mainly in framework of a research grant, supported by GIF with the AP in role of PI. The current proposal suggests a promising possibility to renew this line of research.

1.2 Methodologies

We will use general theory of coherent configurations and association schemes. Diverse tools from computer algebra like GAP, COCO, COCO-II, DISCRETA will be used and modified (see e.g. tutorial T2 by Klin et al in [13] for detailed presentation of the related methodology). An interplay with other existing computer packages (including those developed in Slovenia) is of a great significance. The use of Gröbner bases also provides a promising potential.

2 Information on funding

Though Israel does not get get direct funding in framework of ERS scheme, the authorities of BGU will provide to the AP full logistical support. Research collaborators of the AP are welcome to visit BGU during all 3 years of the project in order to conduct a joint research. It is expected that PIs, related to the parts where the AP will contribute, will provide a partial support of his travel expenses to the corresponding university. We also expect that in a couple of cases the successful impact of tandems, involving AP (like Klin-Macaj, Fowler-Klin) will serve as an extra motivation to apply for new joint grants and thus to get finally direct extra funding.

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