# RESEARCH STATEMENT

Geometric combinatorics stands at the crossroads of rapidly developing areas of research in mathematics. Many current problems in algebraic geometry, representation theory, and theoretical physics share stunning relationships with geometric objects and their combinatorial properties. These relationships, along with problems at the core of discrete geometry, foster the emergence of key mathematical challenges. Coxeter groups are prominent examples of structures that lead to such problems. Coxeter groups have connections in particular with symmetric and inscribable polytopes, hyperplane arrangements, hyperbolic manifolds, and quantum systems. These relations intrigue me ceaselessly! Even more so when I discover connections with other areas of mathematics and when computations and optimization are involved. This summarizes shortly why I am passionate about algebraic combinatorics and discrete geometry and do research in those areas.

Through my international research experiences that took place in dynamic and leading research institutes, I bring together a unique blend of cutting-edge combinatorial, geometric, and large scale computational approaches to investigate algebraic and topological structures. My research interests may be grouped into three main areas. Below, I describe their central open problems and implications, along with how my recent work sparks new research avenues.

## A) GENERALIZED HYPERSIMPLICES IN QUANTUM PHYSICS

Summary. The permutahedron is perhaps the most well-known geometric object related to finite Coxeter groups. Consider the symmetric group  $A_{n-1}$  and its action on  $\mathbb{R}^n$  by permutation of coordinates. The convex hull of the orbit of the point  $(1,2,\ldots,n)$  is the (n-1)-dimensional permutahedron. Taking a different starting point or a different finite Coxeter group leads to various notions of "generalized" permutahedra. Hypersimplices are generalized permutahedra where the starting point is chosen to have entries equal to 0 or 1. Hypersimplices play an important role in quantum physics: the values 0 or 1 represent whether a fermion is present or not in an orbital of a quantum system. Density functional theory is a fundamental computational method that was developed in the 1960's by theoretical physicists to circumvent the difficulties of solving the Schrödinger equation for large quantum systems [HK64]. Around the same time, it has been established that the set of "w-ensemble N-representable 1-particle reduced density matrices" that fulfill the Pauli exclusion principle can be expressed using an hypersimplex, see e.g. [Col63]. This opened the door to the usage of tools from discrete geometry to help in studying quantum systems with many particles [BD72], but went seemingly unnoticed by the geometric combinatorics community until very recently. A better knowledge of interpolation between hypersimplices and permutahedra would enable physicists in the future to calculate more efficiently with higher accuracy excited states, optical gaps and behavior at finite temperature of large quantum states.

Research Plans. The goal of this project is to clarify the role of hypersimplices, permutahedra and their interpolations in quantum physics and to described their combinatorial and geometric structures. Motivated by Schilling's work on reduced density functional theory [Ben+20], the following problem has become of prime importance:

Question. Let 
$$X = \{x^{(j)} \in \mathbb{R}^d\}_{j=1}^k$$
 be a set of  $k$  distinct points such that  $1 \ge x_1^{(j)} \ge x_2^{(j)} \ge \cdots \ge x_d^{(j)} \ge 0$  and  $\sum_{i=1}^d x_i^{(j)} = 1$  for all  $j \in \{1, \ldots, k\}$ . What is the  $H$ -description of the polytope  $P_X := \operatorname{conv}\left(\left\{\pi(x^j) : \pi \in S_d, \ j=1,\ldots,k\right\}\right)$ ?

Solving this problem will permit to establish a generalization of Pauli's exclusion principle from 1925 [SCL20]! This description is a key step in order to make possible the determination of excited states in interacting quantum systems through so-called "1-particle reduced density matrix functional theory". In turn, this would generalize the respective ensemble density functional theory of Pierre Hohenberg and Walter Kohn.

#### B) Geometric Realizations of Subword Complexes of Coxeter Groups

**Summary.** Coxeter groups are abstractions of groups generated by reflections in a vector space. By their simple combinatorial definition, they provide a flexible framework to study internal properties of geometric or topological objects. Among these objects are simplicial complexes called *subword complexes*, which are homeomorphic to balls or spheres. They were introduced in the context of Gröbner geometry of Schubert varieties [KM04].

Through their definition using reduced words, they can be used as an intermediary to translate between geometric and combinatorial concepts. Namely, in [CLS14], Ceballos, Stump and I exposed a strong relationship between subword complexes and cluster complexes in the theory of cluster algebras which led to fruitful research avenues. In particular, subword complexes have shown further connections to cluster algebras [CP15], Hopf algebras [BC17], and many geometric structures [Jon05][SW09][PP12][Esc16][BCL17][BZ19]. On the other hand, the structure of reduced words of Coxeter groups has a dramatic effect on the geometrical realizations of subword complexes as polytopes. At the intersection of algebraic combinatorics and discrete geometry, the following open question resisted for the last 16 years [KM04, Question 6.4]:

Are spherical subword complexes realizable as the boundary of simplicial polytopes?

In the affirmative case, we would say that subword complexes are "polytopal". Around a century ago, Steinitz showed that every 2-dimensional simplicial sphere is polytopal. In higher dimensions, this question is part of "Steinitz' Problem" asking to determine polytopal spheres among all simplicial spheres. The determination of the polytopality of spheres is famously known to be fraught with pitfalls: The determination of the polytopality of a simplicial sphere is known to be an NP-hard problem [Ric96], making progress in this direction continually limited, and for  $d \ge 3$ , as the number of vertices increases, most simplicial d-spheres are not polytopal.

An answer to the above question carries striking consequences: The existence of such polytopes would provide a distinguished family of polytopes with exceptional combinatorial properties and connections to many areas of mathematics, thus opening the door to the use of new discrete geometric tools. On the other hand, if not all subword complexes are polytopal, they would constitute a large and combinatorially simple family of vertex-decomposable simplicial spheres arising *naturally* that *are not* polytopal. This would be of extraordinary interest, as presently such obstructions are usually obtained using brute force enumeration or *ad hoc* constructions. Answering this question would also settle three conjectures simultaneously [KM04][Jon05][SW09] who have seen little progress.

Research Progress. Given an element w of a Coxeter group W, the graph  $\mathcal{G}(w)$  whose vertices are reduced expressions of w and edges represent braid moves between expressions is well-known to be connected [Mat64][Tit69]. Bergeron, Ceballos and I proved that the graph  $\mathcal{G}(w_{\circ})$  and certain minors are bipartite graphs, which is used to derive the first necessary conditions for the polytopality of subword complexes [BCL15]. Using these conditions, we constructed complete simplicial fans for subword complexes of type  $A_3$  and for certain cases in type  $A_4$ .

In [Lab20], I describe explicitly a family of chirotopes that encapsulate the necessary information to obtain geometric realizations of subword complexes. The family of chirotopes is described using certain matrices called "parameter matrices". The key result proven therein is that **parameter matrices are universal**: Their existence combined with conditions in terms of Schur functions is equivalent to the realizability of all subword complexes of this Coxeter group as chirotopes.

Research Plans. Subword complexes encompass objects of such complexity and generality that even a specific case study is difficult. The only tangible approach is the one founded on the exploitation of fundamental principles that polytopes realizing subword complexes must obey. These fundamental

principles are: the realizability of their oriented matroids (equivalently, their chirotopes) and the universality of parameter matrices. The results in my article [Lab20] suggest to study realization spaces of subword complexes using a promising combination of Gale duality and Schur functions. These Schur functions should lead to a combinatorial interpretation of parameter matrices in turn providing a concrete approach to construct the sought polytopes.

### C) Combinatorics, Dynamics, and Geometry of Coxeter Groups

Summary. Coxeter groups form a family of groups rich in related structures. On the one hand, the weak order poset encodes the combinatorial structure of Coxeter groups, and is useful to study the Bruhat order, Hecke algebras, and Kazhdan–Lusztig polynomials. On the other hand, root systems are a prime tool to represent Coxeter groups as reflection groups and many combinatorial aspects of Coxeter groups translate into properties of polytopes associated to root systems. The interplay between root systems and the weak order lead to fascinating relations between combinatorial objects (for example automata and reduced words), algebraic objects (for example semi-simple Lie algebras and hyperbolic groups), and geometric objects (for example billiards trajectories and limit sets).

In contrast with the finite case, the infinite weak order is delicate: it is only a meet-semilattice. However, in my doctoral thesis I showed that it is possible to embed it into a bigger lattice for Coxeter groups of rank  $\leq 3$  [Lab13]. It is further possible to describe the join operation geometrically using the corresponding inversion set and their relative position with respect to the imaginary cone [HL16]. Nevertheless, a better geometric understanding of the weak order is desirable and is subject to two generalizations: The "limit weak order" extends the weak order to infinite reduced words, whereas the "extended weak order" extends the usual weak order to infinite biclosed sets. These generalizations give rise to two conjectures: The first states that the limit weak order is a lattice [LP13, Conjecture 10.3][LT15], and the second states that the extended weak order is a complete ortholattice [Dye19, Conjecture 2.5]. While studying these conjectures, we obtained intriguing fractal-like pictures using Sagemath. They show that roots tend to the isotropic cone of the vector space.

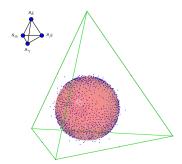


FIGURE 1. The normalized isotropic cone (sphere) and the first thousand normalized roots (dots) for the root system with diagram the complete graph with labels 3.

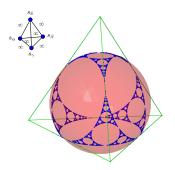


FIGURE 2. The normalized isotropic cone (sphere) and the first thousand normalized roots (dots) for the based root system with diagram the complete graph with labels  $\infty$ .

"Limit roots" were introduced to obtain a geometric understanding of the asymptotic behavior of roots shown in the pictures above [HLR14], and computational and visualization tools were implemented in Sagemath [Lab17]. Limit roots seem to be natural geometric objects allowing to unify the limit weak order and the extended weak order, which both have to be explored in more detail.

Research Progress. Thus far, certain relations between limit roots and other objects have been explained: with sphere packings [CL15], the imaginary cone [DHR16], and Garside theory [DH16]. Limit roots are both geometric through their definition and combinatorial in their close connection to infinite reduced words.

Introduced by Lam and Pylyavskyy, infinite reduced words are right-infinite words with reduced finite prefixes [LP13, LT15]. Given a random vector in a vector space on which a Coxeter group acts, what is the limit set of its orbit? In a joint work with Chen, we characterized these limit sets using eigenspaces of infinite order element in the case of Lorentz spaces [CL17]. We then derived the exact relation between limit roots and infinite reduced words in the Lorentzian case: to each infinite reduced word corresponds a unique limit root. Although very natural, the general relationship between infinite reduced words and limit roots is not yet fully understood.

Research Plans. The goal of this project is to establish and therefore clarify the relation between limit roots and infinite reduced words. The translation between infinite reduced words and limit roots will provide a novel tool for the investigation of boundaries of Coxeter groups. In order to generalize the results from [CL17] to higher ranks, one requires the appropriate equivalence relation on infinite reduced words. The following conjecture makes this equivalence explicit, and motivates this project.

Conjecture (L. 2015). Let (W, S) be a Coxeter system,  $\Phi$  an associated based root system,  $E_{\Phi}$  the set of limit roots,  $W_{\infty}$  the set of infinite reduced words of W, then

$$E_{\Phi} \cong W_{\infty}/\sim$$
,

where  $\sim$  is the relation  $x \sim y$  if and only if  $x = pw_1$  and  $y = pw_2$  where  $w_1$  and  $w_2$  are contained in a common affine Coxeter parabolic subgroup.

The formulation of the conjecture strongly suggest that "subshifts of finite types" are involved and techniques from dynamical systems are key towards a proof. The study of the spectrum of elements is central to prove the conjecture, but the general theory remains to be established [LL15].

A better understanding of non-Lorentzian Coxeter groups would provide many examples which are crucially missing. This motivates to classify further Coxeter groups. When a Coxeter group acts on a Lorentz space, it is called *Lorentzian*. Which Coxeter groups are Lorentzian? In dimension 2, hyperbolic reflection groups were already described by Poincaré and Dyck in the 19<sup>th</sup> century. In dimension 3, Andreev gave four necessary and sufficient conditions expressible as linear inequalities for the existence of an acute-angled polyhedron with a given combinatorial structure which is related to inscribability of polytopes [And70]. In dimensions ≥ 4, things are still far from being completely understood. Vinberg discussed this long standing problem at the ICM in 1983 in Warsaw [Vin84] mentioning "classifying [groups of finite covolume] seems to be an extremely difficult but solvable problem". Based on my work on the classification of "level-2" Coxeter graphs [CL15] and polytope inscribability [Doo+20], I plan to use ideas from Robertson-Seymour's theorem about forbidden minors [RS04], Maxwell's notion of levels of Coxeter graphs [Max82], and tools from real-algebraic geometry to obtain new Lorentzian Coxeter groups.

#### PROJECT-RELATED PUBLICATIONS OF THE AUTHOR

- [SCL20] C. Schilling, F. Castillo, and **J.-P. Labbé**, Comprehensive foundation of one-matrix functional theory for excited states, in preparation (2020) 20 pp.
- [Doo+20] J. Doolittle, **J.-P. Labbé**, C. Lange, R. Sinn, J. Spreer, and G. M. Ziegler, *Combinatorial inscribability obstructions for higher-dimensional polytopes*, Mathematika **66** (2020) no. 4, 927–953.
- [Lab20] **J.-P. Labbé**, Combinatorial foundations for geometric realizations of subword complexes of Coxeter groups, arXiv:2003.02753 (2020) 34 pp. (submitted to Adv. Math.)
- [BCL17] S. B. Brodsky, C. Ceballos, and **J.-P. Labbé**, Cluster algebras of type D<sub>4</sub>, tropical planes, and the positive tropical Grassmannian, Beitr. Algebra Geom. **58** (2017) no. 1, 25–46.
- [CL17] H. Chen and **J.-P. Labbé**, *Limit directions for Lorentzian Coxeter systems*, Groups Geom. Dyn. **11** (2017) no. 2, 469–498.
- [Lab17] J.-P. Labbé, Brocoli: Sagemath package dealing with LImit ROots of COxeter groups, https://github.com/jplab/brocoli (2017) version 1.0.0 3500 lines.
- [HL16] C. Hohlweg and **J.-P. Labbé**, On inversion sets and the weak order in Coxeter groups, European J. Combin. **55** (2016) 1–19.

- [BCL15] N. Bergeron, C. Ceballos, and J.-P. Labbé, Fan realizations of type A subword complexes and multi-associahedra of rank 3, Discrete Comput. Geom. 54 (2015) no. 1, 195–231.
- [CL15] H. Chen and J.-P. Labbé, Lorentzian Coxeter systems and Boyd-Maxwell ball packings, Geom. Dedicata 174 (2015) 43–73.
- [LL15] **J.-P. Labbé** and S. Labbé, A Perron theorem for matrices with negative entries and applications to Coxeter groups, arXiv:1511.04975 (2015) 14 pp.
- [CLS14] C. Ceballos, J.-P. Labbé, and C. Stump, Subword complexes, cluster complexes, and generalized multi-associahedra, J. Algebraic Combin. 39 (2014) no. 1, 17–51.
- [HLR14] C. Hohlweg, J.-P. Labbé, and V. Ripoll, Asymptotical behaviour of roots of infinite Coxeter groups, Canad. J. Math. 66 (2014) no. 2, 323–353.
- [Lab13] J.-P. Labbé. Polyhedral Combinatorics of Coxeter Groups. https://refubium.fu-berlin.de/handle/fub188/628. PhD thesis. Freie Universität Berlin, July 2013, pp. xvi+103.

#### EXTERNAL BIBLIOGRAPHY

- [And 70] E. M. Andreev, Convex polyhedra in Lobachevskii spaces, Mat. Sb. (N.S.) 81 (123) (1970) 445–478.
- [Ben+20] C. L. Benavides-Riveros, J. Wolff, M. A. L. Marques, and C. Schilling, *Reduced Density Matrix Functional Theory for Bosons*, Phys. Rev. Lett. **124** (2020) 180603.
- [BC17] N. Bergeron and C. Ceballos, A Hopf algebra of subword complexes, Adv. Math. 305 (2017) 1163– 1201.
- [BD72] R. E. Borland and K. Dennis, The conditions on the one-matrix for three-body fermion wavefunctions with one-rank equal to six, J. Phys. B 5 (1972) no. 1, 7–15.
- [BZ19] T. Brüstle and J. Zhang, Non-leaving-face property for marked surfaces, Front. Math. China 14 (2019) no. 3, 521–534.
- [CP15] C. Ceballos and V. Pilaud, Denominator vectors and compatibility degrees in cluster algebras of finite type, Trans. Amer. Math. Soc. **367** (2015) no. 2, 755–773.
- [Col63] A. J. Coleman, Structure of fermion density matrices, Rev. Modern Phys. 35 (1963) 668–689.
- [Dye19] M. Dyer, On the weak order of Coxeter groups, Canad. J. Math. 71 (2019) no. 2, 299–336.
- [DH16] M. Dyer and C. Hohlweg, Small roots, low elements, and the weak order in Coxeter groups, Adv. Math. **301** (2016) 739–784.
- [DHR16] M. Dyer, C. Hohlweg, and V. Ripoll, *Imaginary cones and limit roots of infinite Coxeter groups*, Math. Z. **284** (2016) no. 3-4, 715–780.
- [Esc16] L. Escobar, Brick manifolds and toric varieties of brick polytopes, Electron. J. Combin. 23 (2016) no. 2.
- [HK64] P. Hohenberg and W. Kohn, Inhomogeneous electron gas, Phys. Rev. (2) 136 (1964) B864–B871.
- [Jon05] J. Jonsson, Generalized triangulations and diagonal-free subsets of stack polyominoes, J. Comb. Theory, Ser. A 112 (2005) no. 1, 117–142.
- [KM04] A. Knutson and E. Miller, Subword complexes in Coxeter groups, Adv. Math. 184 (2004) no. 1, 161–176.
- [LP13] T. Lam and P. Pylyavskyy, *Total positivity for loop groups II: Chevalley generators*, Transform. Groups **18** (2013) no. 1, 179–231.
- [LT15] T. Lam and A. Thomas, Infinite reduced words and the Tits boundary of a Coxeter group, Int. Math. Res. Not. IMRN (2015) no. 17, 7690–7733.
- [Mat64] H. Matsumoto, Générateurs et relations des groupes de Weyl généralisés, C. R. Acad. Sci. Paris 258 (1964) 3419–3422.
- [Max82] G. Maxwell, Sphere packings and hyperbolic reflection groups, J. Algebra 79 (1982) no. 1, 78–97.
- [PP12] V. Pilaud and M. Pocchiola, Multitriangulations, pseudotriangulations and primitive sorting networks, Discrete Comput. Geom. 48 (2012) no. 1, 142–191.
- [Ric96] J. Richter-Gebert. *Realization spaces of polytopes.* **1643**. Lecture Notes in Mathematics. Springer-Verlag, Berlin, 1996, xii+187.
- [RS04] N. Robertson and P. D. Seymour, *Graph minors. XX. Wagner's conjecture*, J. Combin. Theory Ser. B **92** (2004) no. 2, 325–357.
- [SW09] D. Soll and V. Welker, Type-B generalized triangulations and determinantal ideals, Discrete Math. **309** (2009) no. 9, 2782–2797.
- [Tit69] J. Tits. Le problème des mots dans les groupes de Coxeter. In: Symposia Mathematica (INDAM, Rome, 1967/68), Vol. 1. Academic Press, London, 1969, 175–185.
- [Vin84] E. B. Vinberg. Discrete reflection groups in Lobachevsky spaces. In: Proceedings of the International Congress of Mathematicians, Vol. 1, 2 (Warsaw, 1983). PWN, Warsaw, 1984, 593–601.