Soft Packings, Nested Clusters, and Condensed Matter

Karoly Bezdek, University of Calgary,
Egon Schulte, Northeastern University,
Marjorie Senechal, Smith College

September 29 – October 4, 2019

1 Overview of the subject area of the workshop

Modeling the geometry of condensed matter is a challenging problem. The ongoing revolution in materials science sparked by the discovery of aperiodic crystals in 1982 demands the parallel development of new discrete geometric concepts and tools needed to study aperiodic structures. Thus our workshop was a particularly timely event!

The workshop focussed on "soft packing" and "nested clustering" phenomena in discrete geometric structures and on their applications to unraveling the internal atomic structure of solids and fluids. The classical "building block" model of crystal structure is fast yielding to new models in which nested atomic clusters link and perhaps overlap. However, the nature and geometry of such clusters is currently not well understood. The workshop sought to integrate the theories of tilings, coverings, and packings to address these phenomena and study the underlying mathematical concepts.

We assembled a group of researchers from a broad range of areas in mathematics and other sciences to share recent developments and emerging directions, encourage new collaborative ventures, and build on progress made on specific problems after a recent workshop at the American Mathematical Institute (AIM) and a number of special sessions on this topic. Our group included established researchers and an equal number of junior faculty and students, fostering the synergy between the underlying pure mathematical concepts and the real-world applications. Because our subject matter spans the condensed matter sciences as well as many fields in mathematics, we sought a common language to address concrete open problems, opportunities to discuss ways of solving them, and was of generating further research. Our mix of activities included invited talks, problem sessions, and smaller working groups.

2 Statement of the objectives of the workshop

In 1982, the materials scientist Dan Shechtman shocked the science community with a groundbreaking Â discovery which "fundamentally altered how chemists conceive of solid matter": Â there are crystal-like structures that have x-ray diffraction images exhibiting icosahedral symmetry, which stands in apparent contradiction to the classical "fundamental law" of crystallography that the internal atomic structure of a crystal is periodic and can be described by a lattice. For this profound discovery Shechtman was awarded the 2011 Nobel Prize.

Nowadays the world of crystals includes aperiodic crystals, among them the so-called quasicrystals. Order in crystals is no longer synonymous with periodicity, but exactly what "order" means and how it should be modeled is still debated. For well over a century, geometers and crystallographers have carefully distinguished tilings from coverings and packings, and in particular used tilings to model crystal structure. But the aperiodic crystals whose structures have been explicitly determined cannot be properly modeled by tilings. The basic units in these structures are nested atomic clusters that self-assemble with overlaps and gaps, and also are in motion.

The workshop was centered around the following three major problem areas which are interrelated and arise in applications.

- Nested clustering in aperiodic structures in Euclidean d-space $\mathbb{E}^d$. Structure theory for nested clusters; local rules for building global structures; local characterizations of global structures; and a catalogue of nested clusters.
- Soft sphere packing and its relationship with classical sphere packing. Optimal soft packings; density estimates; and kissing numbers.
- Delaunay (Delone) point sets in $\mathbb{E}^d$. Classification of Delaunay sets; local theory; and geometric structures over Delaunay sets.

Nested clustering

A major focus of this problem area is studying models of "exotic" order in condensed matter (large unit cell crystals and quasicrystals) for clues to their nucleation and growth. This is timely because cluster models are still undeveloped geometrically, and poorly understood physically.

One of us (Marjorie Senechal) had recently been involved in studying the clusters in two specific aperiodic crystals, one experimental and one simulated. (This research was carried out under the AIM Workshop and AIM SQuaRe programs.) Though the geometric descriptions of the clusters in the literature are quite different, reexamining the data her research group found common features that their descriptions in the literature had obscured. It was observed that the same key features had appeared in simulations of dense-packing various solids, including unit balls, in large spheres. This suggested that geometry may play a larger role in the growth of these curious structures than had been thought and will help explain the growth and form of aperiodic crystals more generally. The new approach to the growth of the experimental crystal is presented in [11], leaving open its applicability more generally.

It is expected that similar approaches will shed new light on a large class of complex crystals. The workshop was the ideal place to explore them. This research benefits immensely from interacting with researchers working on soft packings or on Delaunay sets.

Soft packing

As we mentioned above, for well over a century, geometers and crystallographers have carefully distinguished tilings from coverings and packings. What we call soft packings is newer; one of the earliest works in this field is a 1965 paper by L. Fejes Tóth's concerning "Minkowski arrangements of circles". The underlying concept was recently generalized by Böröczky and Szabó. Let $0 < \mu < 1$. Consider a "homogeneous" arrangement $\mathcal{S}$ of (not necessarily congruent) spheres in $\mathbb{E}^d$. Now shrink each sphere S of $\mathcal{S}$ by the factor μ to obtain a new sphere called the μ-kernel of S. Then $\mathcal{S}$ is said to be a Minkowski arrangement of order μ, or a soft packing of order μ, if no sphere of $\mathcal{S}$ overlaps the μ-kernel of another sphere. The main problem is to find the greatest possible (classical) density of Minkowski sphere arrangements of order μ in $\mathbb{E}^d$.

The approach of [2] introduces soft sphere packings in a way that connects traditional sphere packings with sphere coverings, and makes it possible to use the Voronoi tiling method to derive estimates, and extend this method from spheres to nested clusters. A soft packing of spheres of radius $1 + \varepsilon$ is an arrangement of spheres of radius $1 + \varepsilon$ such that the concentric unit spheres form a (hard) Â packing in $\mathbb{E}^d$. The soft sphere packing problem asks for the densest soft sphere packing of radius $1 + \varepsilon$, where the density is the fraction of space covered by the spheres of radius $1 + \varepsilon$. The main open problems include establishing a soft packing analogue of the dodecahedral bound of Hales and McLaughlin, and finding the densest soft sphere packings in 3-space (analogue of the Kepler conjecture).

A related goal concerns analogues of the bounds for the kissing number [1]. The soft kissing number is the maximum number of spheres of radius $1 + \varepsilon$ that can intersect a given sphere of radius $1 + \varepsilon$, subject to the condition that the underlying concentric unit spheres are non-overlapping.

Delaunay Sets

Delaunay sets are point sets in $\mathbb{E}^d$ that are uniformly discrete and relatively dense. These sets provide a convenient framework and common language to address many problems about crystal structures, as the latter are usually described in the language of point sets (atoms, vertices, centers, etc.).

We focussed on the local theory of regular systems (orbits of crystallographic groups) and more general point sets. This theory, initiated by Delaunay in the 1970's, aims at providing a rigorous explanation for the occurrence of global order in a crystalline structure based on the occurrence of congruent patterns. The analysis is carried out in terms of Delaunay sets X of type (r, R), and of ρ-clusters of X (the set of points in X at distance at most ρ from a given point in X). A main goal is to find the regularity radius, the smallest value of ρ such that each Delaunay set X of type (r, R) with mutually congruent ρ-clusters is a regular system; a priori this value depends on d, r and R. We hopes to be able to improve the bounds for ρ. A main goal was to generalize the Local Theorem of [3] (linking the local building blocks with the periodicity of the global structure) to more general point sets.

Another important goal is to expand the classification of Delaunay sets begun by Lagarias [6].

3 Further Developments

Several papers stemming from our workshop are currently at various stages of completion. The authors will, of course, acknowledge their gratitude to BIRS. We will also update the attached bibliography as time goes on.

4 Lectures

The Workshop featured sixteen invited 50-minute lectures on a wide range of topics cutting across several areas. The speakers for each subject area are listed alphabetically.

4.1 Crystals, including quasicrystals

Ron Lifshitz, Tel-Aviv University, gave a lecture about thermodynamic stability of quasicrystals, from fluid dynamics to soft condensed matter. As early as 1985, Landau free-energy models [1-3] and density-functional mean-field theories [4] were introduced in an attempt to explain the stability of quasicrystals, with only partial success if any. It is only in recent years, that great progress has been made in understanding the thermodynamic stability of quasicrystals in such simple isotropic classical field theories. Much of this has happened thanks to insight from the experimental observation of quasicrystalline order in diverse systems ranging from fluid dynamics to soft condensed matter. The key to unlocking the stability puzzle was in the realization that more than a single length scale was required, but more importantly in figuring out how to introduce these multiple scales into the models, and identifying the remaining requirements [5,6]. Lifshitz's team and others have since managed to produce Landau and other mean-field theories with a wide range of quasicrystals as their minimum free-energy states, and have also confirmed some of these theories using molecular dynamics simulations with appropriately designed inter particle potentials [7-12]. The lecture gave a quick overview of the quasicrystals that can be stabilized in these theories—in systems of one or two types of particles, in two and in three dimensions—and attempt to identify a trend that might be emerging in going from Landau theories to more realistic density-functional mean-field theories. It remains an open question whether this trend may eventually lead to understanding the stability of quasicrystals in complex metallic alloys. References relevant to the lecture:

[1] P. Bak, Phys. Rev. Lett. 54, 1517 (1985).

[2] N.D. Mermin, S.M. Troian, Phys. Rev. Lett. 54, 1524 [Erratum on p. 2170] (1985).

[3] P.A. Kalugin, A.Yu. Kitaev, L.C. Levitov, JETP Lett. 41, 145 (1985).

[4] S. Sachdev, D.R. Nelson, Phys. Rev. B 32, 4592 (1985).

[5] R. Lifshitz, H. Diamant. Phil. Mag. 87, 3021 (2007).

[6] R. Lifshitz, D. Petrich, Phys. Rev. Lett. 79, 1261 (1997).

[7] K. Barkan, H. Diamant, R. Lifshitz, Phys. Rev. B 83, 172201 (2011).

[8] A.J. Archer, A.M. Rucklidge, E. Knobloch, Phys. Rev. Lett. 111, 165501 (2013).
[9] K. Barkan, M. Engel, R. Lifshitz, Phys. Rev. Lett. 113, 098304 (2014).
[10] C. V. Achim, M. Schmiedeberg, and H. Löwen, Phys. Rev. Lett. 112, 255501 (2014).
[11] P. Subramanian, A.J. Archer, E. Knobloch, A.M. Rucklidge, Phys. Rev. Lett. 117, 075501 (2016).
[12] S. Savitz, M. Babadi, R. Lifshitz, IUCrJ 5, 247 (2018).
[13] M.C. Walters, P. Subramanian, A.J. Archer, R. Evans, Phys. Rev. E 98, 012606 (2018).
[14] S. Savitz, R. Lifshitz, "Self-assembly of body-centered icosahedral cluster crystals", presentation at this conference (2019).

Jean Taylor, currently at University of California, Berkeley, spoke about "A hunt for new descriptions of old or new 3D quasicrystals with 5-fold symmetry" (a minor revision over the posted lecture title). The project, joint with Marjorie Senechal, comes from a general interest in how crystals grow, especially how quasicrystals grow. In the case of multi-element alloys, it is highly likely to be by formation and then aggregation of clusters. There are many reasons to suspect icosahedral order may be important in forming many clusters; periodicity or quasiperiodicity would then arise from how these local clusters aggregate. Overlapping rhombic triacontahedra (RTs) are central to describing physical crystals with local or global icosahedral symmetry; structures derived from these overlapping RTs are a key to understanding how such crystals might grow and to unifying their presentations. Might overlapping rhombic icosahedra (RIs) also be useful to understanding how crystals and quasicrystals with local or global 5-fold symmetry can be described? Perhaps they could also be a key to how they might grow? Taylor described both their suggestions as to how this might all work out and their search for evidence in physical crystals and quasicrystals.

During the meeting in Oaxaca, Senechal and Taylor essentially settled the questions asked at the end of the previous paragraph. In 2007, Takakura et al, described the Tsai-type Cd-Yb quasicrystal by using overlapping rhombic triacontahedra and golden rhombohedra. Senechal and Taylor found that the idea of band reduction could be applied to their entire icosahedral quasicrystal, to arrive at a fully 5-fold (no stacking) quasicrystal based on overlapping rhombic icosahedra (RIs). Their expectation is that all of our known structures based on overlapping RIs (the periodic one with the same periodicity as an elongated dodecahedron, the periodic stacks and quasiperiodic stacks Taylor found just before the meeting, and their new fully 5-fold) can be obtained by a cut-and-project formalism on a cubic lattice in 6-dimensional space. Furthermore, a likely chemical composition for all of the structures can be hypothesized by analogy with the Takakura et al structure, and a growth mechanism can be hypothesized. All of these structures may be new, or they might be found in materials; they do not know yet. And they still need to compute Fourier transforms so that they will have diffraction patterns to compare.

Erin Teich, University of Michigan, spoke about entropic colloidal crystallization pathways via fluid-fluid transitions and multidimensional prenucleation motifs. The lecture reported about joint work with Sangmin Lee, Michael Engel, and Sharon C. Glotzer. Complex crystallization pathways occur in a variety of systems both in nature and in simulations and experiments. These systems transition from the fluid phase to the solid phase, not via classical nucleation and growth, but rather through the emergence of single or multiple structural precursors in the fluid, which then give rise to the crystallization of the solid phase. The influence of these precursors on the solid phase crystallization, and the structural characteristics of the prenucleation phases, have yet to be fully elucidated. Teich discussed three instances of two-step crystallization of hard-particle fluids, in which crystallization proceeds via a high-density precursor fluid phase with prenucleation motifs in the form of clusters, fibers and layers, and networks, respectively. These are motifs of varying dimension and complexity. The team explores the influence that the dimension of these prenucleation motifs has on the crystallization process, and structurally and dynamically characterizes each crystallization event. The crystals that form are complex, including, notably, a crystal with 432 particles in its cubic unit cell. The results establish the existence of two-step crystallization pathways in entropic systems and showcase the accompanying variety of prenucleation structures that are possible.

Miloslav Torda, University of Liverpool, spoke about dense periodic packings in the light of crystal structure prediction. One of the methods in the design of new materials is to predict the crystal structure of a new compound from its molecular composition. This process involves generating many hypothetical structures based on lattice energy optimization. The lecture presented a different approach based only on the geometry of a molecule with its potential to speed up classical crystal structure prediction computations. The preliminary results with regard to the periodic packing of a geometric representations of the pentacene molecule using

Monte-Carlo molecular dynamic simulations were also shown. Further, the limitations and downsides of the presented approach were discussed, and future directions were proposed.

4.2 Polyhedra, polytopes, and tilings

Nikolai Erokhovets, Steklov Mathematical Institute, Moscow, lectured about the combinatorics and hyperbolic geometry of families of 3-dimensional polytopes, namely fullerenes and right-angled polytopes. The talk studied combinatorial properties of families of simple 3-dimensional polytopes defined by their cyclic and strongly cyclic k-edge-connectivity. Among them are flag polytopes and Pogorelov polytopes, which are polytopes realizable in the Lobachevsky (hyperbolic) space $\mathbb{L}^3$ as bounded polytopes of finite volume with right dihedral angles. The latter class contains fullerenes — simple 3-dimensional polytopes with only pentagonal and hexagonal faces. Erokhovets focussed on combinatorial constructions of families of polytopes from a small set of initial polytopes by a given set of operations. He presented the classical result by V.Eberhard (1891) for all simple 3-polytopes, more recent results by A.Kotzig (1969), D.Barnette (1974, 1977), J.Butler (1974), T.Inoue (2008), and V.D.Volodin (2011), as well as the improvements obtained in his joint work with V.M.Buchstaber (2017-2019). For fullerenes they also have a stronger result. Buchstaber and Erokhovets also studied polytopes realizable in $\mathbb{L}^3$ as polytopes of finite volume with right dihedral angles. Employing E.M. Andreev's theorem (1970), they proved that cutting off ideal vertices defines a one-to-one correspondence with strongly cyclically 4-edge-connected polytopes different from the cube and the pentagonal prism. They showed that any polytope of the latter family is obtained by cutting off a matching of a polytope from the same family or the cube with at most two nonadjacent orthogonal edges cut producing all the quadrangles. The talk described a refinement of D.Barnette's construction of this family of polytopes and gave its applications to right-angled polytopes. Also discussed was a refinement of the construction of ideal right-angled polytopes by edge-twists described in a survey by A.Yu.Vesnin (2017), obtained as a result of employing results by I.Rivin (1996) and G.Brinkmann, S.Greenberg, C.Greenhill, B.D.McKay, R.Thomas, and P.G.Wollan (2005). Its connection with D.Barnette's construction via perfect matchings was also analyzed. Buchstaber and Erokhovets have a conjecture on the behaviour of the volume under operations which would generalize results by T.Inoue (2008), and have some supporting evidence for it.

Dirk Frettloeh, University of Bielefeld, spoke about bounded displacement equivalence in substitution tilings. During the last three decades several results were obtained on bounded displacement equivalence of Delone sets. Two Delone sets are called bounded displacement equivalent if there is a bijection between them such that the distance between any two pairs is bounded by a common constant. (Or more generally: up to scaling). The case of crystallographic Delone sets was settled already in 1991: up to scaling, all crystallographic Delone sets are in the same equivalence class. Hence interesting questions arise about the equivalence of nonperiodic Delone sets. A cute method to produce a large class of nonperiodic Delone sets are tile substitutions. The talk explained the concepts above in detail and presented several results on (non)-equivalence of Delone sets arising from substitution tilings.

Alexey Garber, The University of Texas Rio Grande Valley, spoke about the famous Voronoi conjecture about parallelohedra. Parallelohedra are convex d-polytopes that tile d-dimensional real space $\mathbb{R}^d$ by translation. They establish an important connection between convex polytopes and lattices. The main topic of the lecture was the Voronoi conjecture, a century old conjecture which is still open even though it can be stated in very simple terms. Garber surveyed some known results on the Voronoi conjecture and gave a brief overview about the recent proof of the Voronoi conjecture in five dimensions, in which he was involved. The lecture was based on joint works with M. Dutour-Sikirić, A. Gavrilyuk, A. Magazinov, A. Schürmann, and C. Waldmann.

Marjorie Senechal, Smith College, gave a lecture about parallelohedra, soft packings, and quasicrystals, highlighting surprising connections and perplexing questions. She presented joint work with Jean Taylor and others from their SQuaRE project at the American Institute of Mathematics, San Jose. Building quasicrystal models with Zome tools, the team discovered surprising connections between soft-packed clusters and Federov's famous parallelohedra. Parallelotopes, by definition, tile $\mathbb{R}^n$ by translation and, therefore, their symmetries can only be those of lattices. But if one drops the (sometimes implicit) requirement of convexity, one finds that parallelohedra in $\mathbb{R}^3$ and clusters with "forbidden" icosahedral symmetries interlock. This raises perplexing questions about the role of convexity in the classical parallelotope theory (which was briefly reviewed during the lecture): what, in fact, is that role? And how might one characterize parallelotopes if one drops it? (There is more than one answer to that.) These connections may also shed light on quasicrystal formation, as Jean Taylor explained in her talk.

4.3 Packing and soft packing

Jaeuk Kim, Princeton University, spoke about joint work with Salvatore Torquato about a tessellation-based procedure to construct perfectly hyperuniform disordered packings. Disordered hyperuniform packings (or dispersions) are unusual amorphous states of two-phase materials that are characterized by an anomalous suppression of volume-fraction fluctuations at infinitely long-wavelengths, compared to ordinary disordered materials. While there has been growing interest in disordered hyperuniform materials, a major obstacle has been an inability to produce large samples that are perfectly hyperuniform due to practical limitations of conventional numerical and experimental methods. To overcome these limitations, Kim and Torquato introduced a general theoretical methodology to construct perfectly hyperuniform packings in d-dimensional Euclidean space. Specifically, beginning with an initial general tessellation of space by disjoint cells that meets a "bounded-cell" condition, hard particles are placed inside each cell such that the volume fraction of this cell occupied with these particles becomes identical to the global packing fraction. They proved that the constructed packings with a polydispersity in size are perfectly hyperuniform in the infinite-sample-size limit. The procedure was numerically implemented for two distinct types of initial tessellations; Voronoi and sphere tessellations. For Voronoi tessellations they showed that their algorithm can remarkably convert extremely large nonhyperuniform packings into hyperuniform ones in two and three dimensions. The application to sphere tessellations established the hyperuniformity of the classical Hashin-Shtrikman coated-spheres structures that possess optimal effective transport and elastic properties.

Zsolt Langi, University of Technology, Budapest, discussed soft packings of balls (spheres) in Euclidean spaces. A soft ball packing of unit balls with outer radius $\lambda > 0$ is defined to be a family of pairs of concentric closed balls, one with radius $1 + \lambda$, called a soft ball, and the other one of unit radius, called the core of the soft ball. The talk reviewed results about soft ball packings of unit balls and some related concepts. Most of the results presented were obtained in joint work with K. Bezdek.

Brigitte Servatius, Worcester Polytechnic Institute, lectured about zeolites and tetrahedral packings. Zeolites (zeo = boil; lithos = stone) are microporous, aluminosilicate minerals commonly used as commercial adsorbents and catalysts. In 1973 the book "Zeolite molecular sieves: structure, chemistry and use" (771 pp) by Donald W. Breck appeared. At that time 27 zeolite framework types were known. In 2007, the 6'th edition of the Atlas of Zeolite Framework Types describes 176 known distinct approved types. Zeolites occur naturally but are also produced industrially on a large scale. Combinatorially, zeolites are line graphs of 4-regular graphs and may be finite. However, it is not always possible to realize a combinatorial zeolite as a unit distance graph in 3-space. Mike Winkler found a saturated tetrahedral packing consisting of only 12 tetrahedra. It is not known yet if the packing is rigid. A 16 vertex model was shown to have at least two degrees of freedom. Servatius is suggesting to use Babai's growth rate result for planar locally finite almost vertex transitive graphs to show unit distance embeddability of the line graph of the ball of radius r in the almost vertex-transitive case. The lecture gave an overview of recent results and open problems. Some open problems are listed in the Open Problems section below.

4.4 Periodic frameworks

Bernd Schulze, Lancester University, presented recent progress and open questions about rigidity and flexibility of periodic frameworks. Rigidity Theory is concerned with the rigidity and flexibility analysis of bar-joint frameworks and related constraint systems of geometric objects. This area has a rich history which can be traced back to classical work of Euler, Cauchy and Maxwell on the rigidity of polyhedra and skeletal frames. In the first part of the talk, Schulze gave an introduction to the theory of local and global rigidity of bar-joint frameworks and related structures such as body-bar and body-hinge frameworks, and provided an overview of the key results. In the second part of the talk, Schulze discussed the recent progress on extending these results to infinite periodic frameworks. Schulze also presented some key open questions in this area, some of which have potential applications in crystallography, materials science and condensed matter physics.

Ileana Streinu, Smith College, gave the opening lecture of the workshop and spoke about auxetic behavior in periodic frameworks. In materials science, auxetic behavior refers to the rather unusual property of a material to laterally expand, rather than shrink, when stretched in some direction. Only sporadic examples are known. Streinu presented a brief survey of the geometric theory of auxetic behavior for periodic bar-and-joint frameworks, as introduced in a series of joint recent papers by Ciprian Borcea. The theory leads to new principles for designing an abundance of frameworks that provably support auxetic deformations. It also leads to effective algorithms for deciding when a given framework allows, infinitesimally, an auxetic deformation. Borcea and Streinu have developed code to effectively test for the auxetic property on frameworks built from crystal databases. Streinu concluded with a summary of the current challenges and some preliminary results. The lecture presented joint work with Ciprian Borcea (Rider U.) and Juan Castillo (Harvard U.). Their project was supported by a 2018-19 Harvard Radcliffe IAS Fellowship.

4.5 Discrete point sets

Oleg Musin, The University of Texas Rio Grande Valley, gave a talk about log-optimal spherical configurations, presenting joint work with Peter Dragnev. They enumerated and classified all stationary logarithmic configurations of $d+2$ points on the unit $(d-1)$-sphere in d dimensions. In particular, they showed that the logarithmic energy attains its relative minima at configurations that consist of two orthogonal to each other regular simplices of cardinality m and n, where $m+n=d+2$. The global minimum occurs when $m=n$ if d is even and $m=n+1$ otherwise. This characterizes a new class of configurations that minimize the logarithmic energy on the $(d-1)$-sphere for all d. The other two classes known in the literature, the regular simplex and the cross polytope, are both universally optimal configurations.

Egon Schulte, Northeastern University, talked about the local theory of tilings and Delone sets. Local detection of a global property in a geometric or combinatorial structure is usually a challenging problem. The classical Local Theorem for Tilings says that a tiling of Euclidean d-space is tile-transitive (isohedral) if and only if the large enough neighborhoods of tiles (coronas) satisfy certain conditions. This is closely related to the Local Theorem for Delone Sets, which locally characterizes those sets among uniformly discrete sets in d-space which are orbits under a crystallographic group. Both results are of great interest in crystallography. The lecture discussed old and new results from the local theory of tilings and Delone sets.

4.6 Knots and links

Woden Kusner, Vanderbilt University, gave a lecture about Gordian unlinks. Given a sufficiently nice embedded space curve, one can thicken it into a physical rope. A pair of physical configurations is Gordian if there is no physical isotopy that takes one to the other. It is an (old) open problem to describe a Gordian unknot. The lecture explored some special configurations of physical links by considering extrusion along with various packing constraints. This is a dual perspective to the topological sweep-out procedure Coward and Hass used to first describe a Gordian split link. There are some advantages that appear with this shifted view; one trades a general statement about knots and surfaces for tighter area bounds and rigidity, severely constraining the character of certain physical isotopies. In the end, as Kusner showed, this is sufficient to describe a Gordian Unlink. This work is related to joint work with Rob Kusner and Greg Buck.

5 Problem Session

The Workshop's Problem Session provided the opportunity to present new and old problems and discuss their status.

Problems on tilings of the unit disk $\mathbb{B}^2$ (Á. Kurusa, Z. Langi and V. Vígh)

In recreational mathematics the following problem seems to regularly resurface from time to time: Find a monohedral tiling of the closed Euclidean unit disk $\mathbb{B}^2$ (i.e. a tiling in which all tiles are congruent) such that the center o of the disk does not belong to all tiles. The best known example is a tiling with 12 tiles, which, incidentally, was chosen as the emblem of the Mathematics Advanced Study Semesters (MASS) program at Pennsylvania State University. On the other hand, it is fairly easy to see that no such tiling exists with only two tiles [1]. This inspired the following two problems.

PROBLEM 1. *What is the smallest number $n(\mathbb{B}^2)$ such that there is a monohedral tiling of $\mathbb{B}^2$ with $n(\mathbb{B}^2)$ topological disks as tiles in which the center o of $\mathbb{B}^2$ does not belong to all tiles. In addition, are there monohedral tilings of the closed Euclidean unit d-ball $\mathbb{B}^d$, where $d \geq 3$, with topological balls as tiles in which the center o does not belong to all tiles?*

PROBLEM 2. *Assume that C is a topological disk such that the closed Euclidean unit disk $\mathbf{B}^2$ has a tiling $\mathcal{F}$ consisting of finitely many similar copies of C.*

- *Is it true that $\mathbf{B}^2$ has a tiling $\mathcal{F}'$ consisting of finitely many similar copies of C which are pairwise congruent?*
- *Is it true that $\mathcal{F}$ contains only pairwise congruent tiles?*

References

[1] A. Belov, R. Fedorov and A. Kovaldzhi (eds.), Moscow Mathematical Olympiads, 2000-2005, MSRI, Berkeley, CA; AMS, Providence, RI, 2011.

Problem on Koebe polyhedra (Zsolt Langi)

A theorem of Brightwell and Scheinermann [1] states that every combinatorial class of convex polyhedra in Euclidean 3-space $\mathbb{R}^3$ contains a representative all of whose edges are tangent to the unit sphere $\mathbb{S}^2$ centered at the origin o, and this representative is unique up to Möbius transformations. These representatives of the combinatorial classes are called Koebe polyhedra. Springborn [2] gave a proof that in every combinatorial class of convex polyhedra there is a Koebe polyhedron with the property that the barycenter of the tangency points on its edges is the origin o, and this polyhedron is unique up to isometries of $\mathbb{R}^3$. Lángi [3] proved that apart from uniqueness, Springborn's result remains true if we replace the barycenter of the tangency points by any of the following:

- center of mass of the k-skeleton of the Koebe polyhedron, where $k = 0, 1, 2$;
- circumcenter,
- one of the incenters,
- if the polyhedron is simplicial, the circumcenter of mass of the polyhedron.

PROBLEM. *Prove or disprove that every combinatorial class of convex polyhedra contains a Koebe polyhedron whose center of mass (assuming uniform density) is the origin.*

References

[1] G.R. Brightwell and E.R. Scheinerman, Representations of planar graphs, SIAM J. Discrete Math. 6 (1993), 214-229.
[2] B.A. Springborn, A unique representation of polyhedral types. Centering via Möbius transformations, Math. Z. 249 (2005), 513-517.
[3] Z. Lángi, Centering Koebe polyhedra via Möbius transformations, arXiv:1804.07572 [math.MG], [math-DS], [math.GT], April 20, 2018.

Problems on zeolites (Brigitte Servatius)

The following problems on zeolites are related to Brigitte Servatius lecture (see above).

PROBLEM 1. *Does there exist a finite 2D zeolite with a planar unit distance realization and having no non-simplex triangle?*

PROBLEM 2. *Do there exist finite non-interpenetrating zeolites with unit distance plane non-rigid realizations?*

PROBLEM 3. *Does it help to take line graphs of unit distance graphs, respectively line graphs of (realizable) line graphs to obtain realizable combinatorial zeolites?*

PROBLEM 4. *Use the special properties of planar 2D zeolites to design "nano-lentils".*

Problems on equal-area triangulations (Bernd Schulze)

We define a *triangulation* of the unit square $[0,1]^2$ in the Euclidean plane to be a triangulation of $[0,1]^2$ with the property that the intersection of any two triangles in the triangulation, if non-empty, is either a common vertex or two vertices and the entire edge that joins them. We do allow vertices to lie on the edges of the square. An *equal-area triangulation* of $[0,1]^2$ is a triangulation of $[0,1]^2$ whose triangles all have the same area.

An open problem (due to R. Kenyon) is to decide whether there exists an $n \in \mathbb{N}$ such that $[0,1]^2$ has infinitely many equal-area triangulations with n triangles.

It is a celebrated result of Paul Monsky that any equal-area triangulation of $[0,1]^2$ must have an even number of triangles [2]. Therefore, we may assume that n is even in the problem above. Since there are only finitely many combinatorial types of triangulations of $[0,1]^2$ for any given number n of triangles, the question above can be rephrased as follows:

PROBLEM. Does there exist an equal-area triangulation of $[0,1]^2$ that is not 'area-rigid' (in the sense that the vertices of the triangles can be moved continuously without changing the combinatorial type of the triangulation and without changing the area of any triangle)?

A related question (originally asked by G.M. Ziegler in 2003) is the following: given an odd number $n \in \mathbb{N}$, how small can the difference between the smallest and the largest area in a triangulation of a square into n triangles become? In other words, if for a triangulation T of $[0,1]^2$ into n triangles with areas $a_1, \dots, a_n$ we define

$$R(T) = \max_{1 \le i < j \le n} |a_i - a_j|$$

then we are interested in

$$\Delta(n) = \min\{R(T) \,|\, T \text{ is a triangulation of } [0,1]^2 \text{ with } n \text{ triangles}\}.$$

The currently best bound is $\Delta(n) = O(\frac{1}{n^3})$ (see [3]). However, it is likely that this bound can be improved significantly. In a recent paper by J.-P. Labbé, G. Rote and G.M. Ziegler [1], a better bound was established for dissections of $[0,1]^2$ (i.e. sets of triangles with disjoint interiors that cover $[0,1]^2$), but not for triangulations of $[0,1]^2$.

References

[1] J.-P. Labbé, G. Rote, and G.M. Ziegler, Area difference bounds for dissections of a square into an odd number of triangles, Experimental Mathematics, 1–23, 2018.

[2] P. Monsky, On dividing a square into triangles, American Mathematical Monthly 77, 161–164, 1970.

[3] B. Schulze, On the area discrepancy of triangulations of squares and trapezoids, The Electronic Journal of Combinatorics 18 (1), P137, 1–16, 2011.

Problems on tilings by combinatorial icosahedra (Egon Schulte)

The following two problems ask about tilings of 3-space $\mathbb{E}^3$ with (convex) combinatorial icosahedra. A tiling of $\mathbb{E}^3$ by convex polytopes is called *normal* if its tiles are uniformly bounded (that is, their inradii are bounded from below, and the circumradii are bounded from above).

PROBLEM 1. Is there a normal tiling of $\mathbb{E}^3$ by convex polytopes all combinatorially isomorphic to the icosahedron?

Variants of this problem may ask for the tiling to be *face-to-face*, meaning that any two tiles meet, if at all, in a vertex, an edge or a 2-face of both. By an old result of Grünbaum and Shephard, any simplicial 3-polytope P (with triangular 2-faces) admits a face-to-face tiling of $\mathbb{E}^3$ by convex polytopes isomorphic to P, and so does the icosahedron. The problem is the normality, which cannot always be achieved but may be possible for the icosahedron.

PROBLEM 2. Is there a tiling of $\mathbb{E}^3$ by convex polytopes, again all combinatorially isomorphic to the icosahedron, such that there are only finitely many congruence classes of tiles.

Similar questions can also be asked for other convex polyhedra. Tilings with polyhedral tiles of just one combinatorial type are called "monotypic" [1]. For the dodecahedron there are monotypic face-to-face tilings with finitely many congruence classes, so the answers to both problems would be positive in this case.

References

[1] E. Schulte, Tilings. Chapter in "Handbook of Convex Geometry" (eds. J.M.Wills and P.Gruber), Elsevier Science Publishers (Amsterdam, 1993), 899–932.

Problems on tilings by equal-area hexagons (Dirk Frettlöh)

The following problem on hexagonal tilings was posed, and subsequently solved at the Workshop by Dirk Frettlöh, Alexey Glazyrin and Zsolt Langi [1]. The abstract of [1] is included.

PROBLEM. Is there a tiling of $\mathbb{E}^2$ by convex hexagons of unit area and bounded perimeter, which is not vertex-to-vertex at more than k vertices, $k \geq 2$.

References

[1] D. Frettlöh, A. Glazyrin, Z. Langi, Hexagon tilings of the plane that are not edge-to-edge, arXiv:1911.12752 [math.MG].

Abstract. *An irregular vertex in a tiling by polygons is a vertex of one tile and belongs to the interior of an edge of another tile. In this paper we show that for any integer $k \geq 3$, there exists a normal tiling of the Euclidean plane by convex hexagons of unit area with exactly k irregular vertices. Using the same approach we show that there are normal edge-to-edge tilings of the plane by hexagons of unit area and exactly k many n-gons $(n > 6)$ of unit area. A result of Akopyan yields an upper bound for k depending on the maximal diameter and minimum area of the tiles. Our result complements this with a lower bound for the extremal case, thus showing that Akopyan's bound is asymptotically tight.*

Concluding we list some relevant general references. See also the references specific to lectures or open problems listed earlier.

General References

[1] I.A.Baburin, M.Bouniaev, N.Dolbilin, N.Y.Erokhovets, A.Garber, S.V.Krivovichev, and E. Schulte, On the Origin of Crystallinity: a Lower Bound for the Regularity Radius of Delone Sets, *Acta Crystallographica* **A74** (2018), 616–629.

[2] K. Bezdek, *Lectures on Sphere Arrangements - the Discrete Geometric Side*, Fields Institute Monographs, **32**, Springer, NY, 2013.

[3] K. Bezdek and Z. Lángi, Density Bounds for Outer Parallel Domains of Unit Ball Packings, *Proc. Steklov Inst. Math.* **288** (2015), 209–225.

[4] B.N. Delaunay, N. Dolbilin, M. Shtogrin, and R. Galiulin, A local criterion for regularity of a system of points, *Sov. Math. Dokl.* **17** (1976), 319–322.

[5] M. Engel, P.F. Damasceno, C. L. Phillips, and S.C. Glotzer, Computational self-assembly of a one-component icosahedral quasicrystal, *Nature Materials* **14** (2015), 109–116.

[6] T.C. Hales, A proof of the Kepler conjecture, *Ann. Math.* **162/3** (2005), 1065–1185.

[7] J. Lagarias, Geometric Models for Quasicrystals, I, II, *Discrete Comp. Geom.* **21** (1999), 161–191 and 345–372.

[8] O. Musin, The kissing number in four dimensions, *Ann. Math.* **168** (2008), 1–32.

[9] D. Pellicer and E. Schulte, Regular polygonal complexes in space, I, II, *Trans. Amer. Math. Soc.* **362** (2010), 6679–6714 and 365 (2013), 2031–2061.

[10] E. Schulte, Polyhedra, complexes, nets and symmetry. *Acta Crystallographica Section A* 70 (2014), 203–216.

[11] M. Senechal, Delone Sets and Condensed Matter: the dialogue continues, *Proc. Steklov Inst. Math.* **288** (2015),1–6.

[12] M. Senechal and J. Taylor, Quasicrystals: the view from Stockholm, *Math. Intelligencer* **35** (2013), 1–9.

[13] J.E. Taylor, E.G. Teich, P.F. Damasceno, Y. Kallus, and M. Senechal: On the Form and Growth of Complex Crystals – The Case of Tsai-Type Clusters, *Symmetry* **9(9)** (2017), 188–200.