Quasicrystals: pattern formation and aperiodic order

4 – 8 June 2018
International Centre for Mathematical Sciences, Edinburgh

Abstracts

Baake, Michael
Spectral notions of aperiodic order
Various notions of spectra are in use in the theory of aperiodic order, including diffraction, dynamical and operator spectra. All have their justification, while their mutual relations are only partially understood.

In this introductory talk, some aspects will be recalled, with emphasis on the pair correlation approach to diffraction and dynamical spectra. In particular, we will consider pair correlations of primitive inflation rules and how they can be used to assess the spectral type. While this talk will focus on one-dimensional systems, the contribution by Franz Gähler will augment this with higher-dimensional tiling examples.

Dotera, Tomonari
Bronze-mean quasiperiodic tiling and its extensions
Quasicrystals are believed to have non-traditional crystallographic symmetry such as icosahedral, decagonal, dodecagonal, and octagonal rotational symmetries. Indeed, quasiperiodicity is characterized by two or more spacings whose length ratio is an irrational number associated with the unconventional rotational symmetry: for instance, the golden mean Penrose tiling with decagonal symmetry and the silver mean Ammann–Beenker tiling with octagonal symmetry. Contrary to the belief that quasicrystals are originated from the unusual rotational symmetries, we present a "6-fold" self-similar quasiperiodic tiling related to the "bronze mean", which number is a natural extension in the literature. Using a two-lengthscale potential, which has turned out to be a minimal and efficient tool to produce quasicrystals, we have obtained a random-tiling of the bronze-mean quasicrystal [1,2]. In this presentation, we further present an infinite series of metallic-mean and 6-fold self-similar quasiperiodic tilings associated with the bronze-mean tiling.

[1] Dotera, T., Oshiro, T. & Ziherl, P. (2014). Nature 506, 208-211, doi:10.1038/nature12938.
[2] Dotera, T., Bekku, S. & Ziherl, P. (2017). Nature Materials, 16, 987-992 (2017). doi:10.1038/nmat4963

Dulle, Martin
Quasicrystals from star shaped polymer micelles
Quasicrystals in soft matter systems are still a rare occurrence and the underlying principles of formation are still not well understood. Recent work from groups either working with block-copolymer melts or POSS headed PS chains as well as MD-simulation concluded that the formation of Frank-Kasper and or quasicrystalline phases has to involve the partition of the self-assembly structures into two species with different aggregation numbers. These findings suggest that no true one component system is capable of forming quasicrystals.

Here we show with MD-simulations that a true single component system with an isotropic and experimentally proven pair potential can even form an icosahedral type 3D quasicrystal as well as Frank-Kasper and dodecagonal quasicrystalline phases. The well-known purely repulsive logarithmic pair potential of Pinkus and Witten was used to describe the interaction forces between our star shaped micelles at high volume fractions. With the simulations we were able to replicate the phases we found experimentally and also the transition from a fcc crystal to a dodecagonal quasicrystal. Because the pair potential is not limited to a single type of polymer it opens the possibility to produce quasicrystals from a multitude of block-copolymers or composite materials in a systematic way.

Edagawa, Keiichi

Growth mechanism of quasicrystals

Quasicrystals possess quasiperiodicity, where the structure cannot be described simply by the repetition of a unit cell like conventional crystals. This fact raises the question of how quasicrystals grow, i.e., what physical mechanism makes the growth of quasicrystals possible. While crystals can grow by copying a unit cell via local atomic interactions, nonlocal structural information seems to be required in the growth of quasicrystals. This problem has attracted much attention ever since the first discovery of a quasicrystal in 1984, and has been discussed frequently mainly from the theoretical points of view. Onoda et al.[1] found that there exists local rules that enable the growth of the 2D Penrose tiling. Until recently, the growth mechanism according to such local rules have been widely believed as a plausible model of quasicrystal growth. However, our recent in-situ observations [2] of the growth process of a quasicrystal suggested the possibility of a growth mechanism different from the model. In our experiments, the introduction of phason defects and repair of them afterwards were frequently observed during growth. Here, tile rearrangements to repair defects were observed in a large area including not only newly grown parts near the growth front but also already grown parts far inside the growth front. This is not consistent with an ideal growth according to elaborate local rules like those in Onoda's model.
In this talk, we will discuss the growth mechanism of quasicrystals on the basis of the simulation results we have recently conducted by use of numerical models of Engel et al. [3]

1. G.Y. Onoda et al., Phys. Rev. Lett. 60 (1988) 2653.
2. K. Nagao et al., Phys. Rev. Lett. 115 (2015) 075501.
3. M. Engel et al., Nat. Mater. 14 (2015) 109.

Engel, Michael

Icosahedral quasicrystals in simulation

Quasicrystals with icosahedral symmetry are the only types of quasicrystal that are aperiodic in all directions. An icosahedral quasicrystal has been the first quasicrystal to be discovered in nature in 1982 and icosahedral quasicrystals remain, arguably, the least understood. The inherently three-dimensional nature of their tiling complicates structure solution in alloys and the fact that they have not been found in soft matter means it is impossible to study them on larger length scales. However, there have been recent reports of icosahedral quasicrystals in simulation, where we have direct access to particle coordinates and trajectories. In this contribution, I will review recent discoveries of icosahedral quasicrystals in one-component systems of particles. I will discuss geometric and numerical methods to study icosahedral quasicrystals in simulation and apply them to analyze the structure and dynamics of observed quasicrystals. I will close with implications for stabilization mechanisms for icosahedral order.

Gähler, Franz

Absence of absolutely continuous diffraction spectrum in inflation tilings

Recently, we have developed exact renormalisation equations for the pair correlations of inflation tilings (see the talk of M. Baake).

The Fourier transform of these determine the diffraction spectrum of the tiling. As the correlations responsible for the absolutely continuous (ac) part of the spectrum must satisfy the renormalisation equations separately, conditions on the existence of a non-trivial ac part in the diffraction can be derived. This allows to exclude an ac part in many cases. We illustrate this technique with a number of examples in one and two dimensions, where such a result was not previously known.

Galanov, Ilya
On self-assembly of aperiodic tilings
Aperiodic tilings serve as a mathematical model for quasicrystals, such crystals that don't have any translational symmetry (Penrose tiling is one famous example). The question is how to grow such a tiling just by adding tiles one by one using only the local information (the motivation is to mimic the growth of a real world quasicrystals). In this talk we will propose a local growth algorithm for a particular class of aperiodic tilings (cut-and-project tilings of finite type). We will illustrates this on two examples (namely the Penrose tiling and the Golden-Octagonal tiling).

Hirvonen, Petri
Growth and characterization of two-dimensional poly(quasi)crystals
We use a simple two-mode phase field crystal (PFC) model to simulate grain growth in realistic two-dimensional model systems of square and hexagonal, as well as of 10- and 12-fold symmetric quasicrystal lattice symmetries. Modelling the evolution of poly(quasi)crystals had remained a challenge until the arrival of PFC, giving access to long diffusive time scales. We characterize the model systems using a powerful new method for segmenting and analyzing grain structures. This method generalizes effortlessly to all lattice types of even-fold rotational symmetry. To our knowledge, our7 characterization method is the first of its kind so far for quasicrystals.

Iooss, Gérard
Quasipattern locking in the superposition of two periodic patterns
We consider a quasilattice built from the superposition of two hexagonal lattices, making a small angle $alpha$ between them. We prove that there are in general 2 or 3 different steady bifurcating quasipatterns solutions, invariant under rotations of angle $\pi/3$, for the Swift–Hohenberg PDE model. The first two solutions come naturally from the addition at first order of the two classical hexagonal patterns. A third solution appears when the angle α takes values $p\ \pi/q$ with q odd number. In such cases, the smallest order when a quasiperiodic term appears is $\varepsilon^{q'-2}$, where $q' = q$ if 3 does not divide q, while $q' = q/3$ if 3 divides q. When α is not of this form, there still also exist the two periodic hexagonal patterns and the new "exotic" solution appearing for the $\alpha \in \mathbb{Q}\pi$ mentioned above, differs only at a very high order in general, from one of the periodic solution. This might be interpreted as a "pattern locking" when α varies. (Joint work with S. Fauve)

Jiang, Kai and Zhang, Pingwen
Quasicrystals: numerical methods and applications
Quasicrystals are important ordered structures in materials. Compared with periodic crystal, quasicrystals do not possess translational symmetry, but have orientational symmetry. After about 30 years of during efforts, a lot of problems, such as the position of the quasi-lattice sites, the diffraction of quasicrystals, have been solved. However, there still exist unsolved problems, such as the stability of quasicrystals, the difference between soft- and hard-quasicrystals. Solving these problems requires the combination of physical understanding, mathematical analysis, and novel computational methods. In this talk, we will give a short review about the numerical methods for quasicrystals, and introduce our projection method and its applications to a class of coarse-grained phase field crystal models with two scales.

Knobloch, Edgar
From periodic patterns to quasiperiodic patterns
In this talk I will describe techniques for constructing amplitude equations describing weakly nonlinear periodic patterns in two and three dimensions near a spontaneous symmetry breaking

bifurcation of a homogeneous state, and their stability. I will also discuss how these equations are modified in the presence of a conserved quantity and (less rigorously) for nonperiodic patterns such as quasipatterns.

I will conclude with examples of computations of both spatially extended and spatially localized quasicrystals from a phase field crystal model.

Lifshitz, Ron

Multiple-scale structures: from Faraday waves to soft-matter quasicrystals

For many years, quasicrystals were observed only as solid-state metallic alloys, yet current research is now actively exploring their formation in a variety of soft materials, including systems of macromolecules, nanoparticles and colloids. Much effort is being invested in understanding the thermodynamic properties of these soft-matter quasicrystals in order to predict and possibly control the structures that form, and hopefully to shed light on the broader yet unresolved general questions of quasicrystal formation and stability. Moreover, the ability to control the self-assembly of soft quasicrystals may contribute to the development of novel photonics or other applications based on self-assembled metamaterials. Here a path is followed, leading to quantitative stability predictions, that starts with a model developed two decades ago [1] to treat the formation of multiple-scale quasiperiodic Faraday waves (standing wave patterns in vibrating fluid surfaces) and which was later mapped onto systems of soft particles, interacting via multiple-scale pair potentials [2,3]. The presentation reviews, and substantially expands, the quantitative predictions of these models, while correcting a few discrepancies in earlier calculations, and presents new analytical methods for treating the models [4]. In so doing, a number of new stable quasicrystalline structures are found with octagonal, octadecagonal and higher-order symmetries, some of which may, it is hoped, be observed in future experiments.

Some references:

1. R. Lifshitz, D. Petrich, Phys. Rev. Lett., 79, (1997), 1261-1264.
2. K. Barkan, H. Diamant, R. Lifshitz, Phys. Rev. B, 83, (2011), 172201.
3. K. Barkan, M. Engel, R. Lifshitz, Phys. Rev. Lett., 113, (2014), 098304.
4. S. Savitz, M. Babadi, R. Lifshitz, IUCrJ, 5, (2018), 247-268.

Mahanthappa, Mahesh K

Amphiphile self-assembly into lyotropic liquid crystalline Frank-Kasper phases and liquid quasicrystalline states

Minimally hydrated amphiphiles self-assemble into lyotropic liquid crystals (LLCs), which exhibit periodic aqueous and hydrophobic nanodomains. Commonly observed lyotropic mesophases include 1D lamellae, 2D columnar phases, 3D bi-continuous networks, and high symmetry 3D sphere packings. Based on hard sphere packings, spherical micelles are intuitively expected to form high symmetry body-centered cubic, face-centered cubic, and hexagonally close-packed structures. However, we recently discovered ionic surfactant micelles can spontaneously produce low symmetry, tetrahedrally close-packed Frank-Kasper (FK) sigma and A15 phases, related C14 and C15 Laves phases, and even dodecagonal quasicrystals (DDQCs). These new, low symmetry phases arise from a frustrated thermodynamic balance that minimizes local variations in amphiphile solvation, while maximizing global micelle cohesion within the ensemble. We will focus on how surfactant structure dictates lyotropic sphere packing symmetry selection and the thermodynamics of these complex assemblies. Analogies between symmetry breaking in metal crystals and these self-assembled soft materials will be discussed.

Sadun, Lorenzo

Tiling cohomology

In this talk I will go over various aspects of tiling cohomology. The technical definition of Cech cohomology is needlessly complicated for our purposes. Instead, I'll explain how to visualize tiling cohomology with pattern-equivariant cochains, how to compute tiling cohomology via inverse limits, and how tiling cohomology (especially H^1) is used to understand shape changes, homeomorphisms of tiling spaces, and, if time permits, rotation "numbers".

Schmiedeberg, Michael

Growth of soft quasicrystals

By employing a phase field crystal model for quasicrystals we explore how a quasicrystal grows. We observe two different growth modes. Close to the triple point a perfect, defect-free quasicrystal can grow. However, far away from the triple pint the growth is dominated by phasonic flips which are incorporated as local defects into the grown structure [1]. The later structure corresponds to a dislocation-free random-tiling-like quasicrystal.

A similar behaviour is found for Brownian dynamics simulations of the growth front of a quasicrystal. Depending on the growth rate and the mobility of the particles close to the front, either excitation-free quasicrystals or random-tiling-like structures can be found.

Finally, we explore how the growth started by multiple seeds is affected by the possibility of stress relaxation via the phasonic degrees of freedom [2].

[1] C.V. Achim, M. Schmiedeberg, H. Löwen, Phys. Rev. Lett. 112, 255501 (2014).
[2] M. Schmiedeberg, C.V. Achim, J. Hielscher, S. Kapfer, and H. Löwen, Phy. Rev. E 96, 012602 (2017)

Socolar, Joshua

Formation of limit-periodic structure

Tiling theory reveals that systems of particles with local interactions can have limit-periodic ground states. Perhaps the simplest example in a 2D lattice model based on the Taylor–Socolar tiling. The system reaches the ground state via a slow quench through an infinite sequence of phase transitions. Surprisingly, the same state can be reached by models in some parameter regimes where the true ground state a crystal. I will describe these models and a 3D generalization of the Taylor–Socolar tiling, explain how limit-periodic structure emerges in them, and discuss open questions regarding possible material realizations.

Strungaru, Nicolae

Meyer sets and their diffraction

In this talk we review the definition and basic properties of Meyer sets. We show that the diffraction pattern of a Meyer set has many Bragg peaks, which are highly ordered, and that each of the absolutely and singularly continuous spectrum is either trivial or has relatively dense support. If the time permits, we also discuss the connection between the diffraction formula for Meyer sets and the Poisson Summation Formula for the lattice of the related cut and project scheme(s).

Walton, Jamie

Resurrecting the space group of an aperiodic pattern

A periodic pattern of Euclidean space is completely determined, up to "locally reversible redecorations", by its space group of global symmetries. For an aperiodically ordered pattern the group of global symmetries is not a particularly enlightening object: the interesting thing about aperiodically ordered patterns is that they can have a rich structure of internal symmetries whilst having very few (if any) global symmetries. In this talk I shall discuss recent work with John Hunton which expresses the space group of a periodic pattern via a topological route. These rotational topological invariants can be applied to periodic as well as non-periodic patterns, which suggests that they are one approach to defining the analogue of the space group, or of its invariants, for an aperiodic pattern.

Yassawi, Reem
Substitutions and linear cellular automata
We describe the relationship between substitutions of constant length and mixing shapes for linear cellular automata. (Joint work with Robert Fokkink).

Zeng, Xiangbing
Micellar and columnar liquid quasicrystals and their tiling rules
Recent advances on the experimental observation, by high resolution AFM and Grazing Incidence XRD, of liquid quasicrystals (LQCs) with 12-fold rotational symmetry will be discussed. Such LQCs are observed in two kinds of systems, by packing of either dendrons self-assembled from dendrons, or columns with polygonal cross-sections from T- and X-shaped molecules. The results suggest that the 12-fold symmetry in such systems is most likely resulted from a random tiling of triangles and squares. Related structures of approximants of the LQC phases will be presented too.

POSTERS

Nakakura, Joichiro
POSTER: *Associated tilings derived from the bronze-mean quasicrystal*

Savitz, Samuel
POSTER: *High-Dimensional ADE Crystal Stability, the E_8 Band Structure, and its 30-fold Quasicrystal* (joint with Marcus Bintz)

Savitz, Samuel
POSTER: *Thermodynamic Stability of the Leech Lattice and the Crucially Chiral 46-fold Quasicrystal in its Band Structure*

Subramanian, Priya; Archer, Andrew; Knobloch, Edgar; Rucklidge, Alastair
POSTER: *Spatially extended and localized quasicrystals in 2D and 3D*