Almost periodic order: spectral, dynamical, and stochastic approaches

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1 Overview of the Field

Quasicrystals were discovered in early 1982 by Dan Shechtman (Haifa) in the form of an AlMn alloy that displayed a sharp Bragg type diffraction image with perfect icosahedral point symmetry. This challenged the understanding of solids at the time, and needed a while to be accepted for publication [16]. Ultimately, it led to a paradigm shift for what we understand as 'order' in a solid or in a more general structure. For this discovery, Shechtman was awarded the Nobel Prize in Chemistry in 2011, just a few days after our meeting took place.

The field of Aperiodic Order is the mathematical counterpart to the physics and chemistry of quasicrystals, and the meeting was concerned with all aspects of it that relate to almost periodicity. In fact, the experimental discovery by Shechtman had many precursors in mathematics, ranging from ornaments via Kepler's famous fivefold pattern and Penrose's tiling to modern tiling theory, or from Bohr's theory of almost periodic functions via Meyer's book [13] to the present day development of almost periodic measures.

2 Recent Developments and Open Problems

The field has seen substantial recent developments in several directions. Specifically, we single out the following three:

- The theory of point processes has transformed the field of mathematical diffraction theory (see [3] for a recent review). This has allowed for treatment of various random models as well as a solution to homometry problem for pure point diffraction.

- In the spectral theory of associated Schrödinger operators, an in depth analysis of fractal spectral features of the Fibonacci Hamiltonian has been accomplished.

- Various methods from dynamical systems have provided new perspectives on old problems.

These topics have been a special focus of attention at the conference. They will be discussed in further detail in the next section.

3 Presentation Highlights

3.1 Random Operators: A Short (Hi)Story (Peter Stollmann)

This review talk was about random Schrödinger operators and their history:

- The Anderson model.
- The metal-insulator transition in spectral terms.
- The general formalism of random operators.
- Models with aperiodic order.

While the first sections concentrated on random models and the localization phenomenon, we mentioned in the last section results that treat aperiodically ordered models.

In his celebrated article [1] from 1958, P.W. Anderson proposed a mathematical model to explain the phase transition from insulator to metal in disordered solids. This has prompted intensive research both in mathematics and physics. Despite great progress, the state of the mathematically rigorous understanding of the metal insulator transition is still unsatisfactory: while there are now methods to prove that typical random models exhibit an energy interval with localization (pure point spectrum with rapidely decaying eigenfunctions), there is no rigorous proof of delocalization so far.

The situation is even harder for Hamiltonians that might be used to model quasicrystals. Apart from one-dimensional results, there is little understanding. It is expected that such models will have purely singular continuous spectrum.

3.2 Geometric realization for hyperbolic substitution tilings and an n-dimensional Pisot substitution conjecture (Marcy Barge)

Suppose that Φ is an n-dimensional substitution (non-periodic, primitive, FLC) with linear expansion Λ and tiling space Ω_Φ. We seek a *geometric realization* $G : \Omega_\Phi \to \mathbb{T}^D$ that semi-conjugates the inflation-and-substitution homeomorphism Φ on Ω_Φ with a hyperbolic toral automorphism F restricted to an invariant set of the torus $\mathbb{T}^D$. G should be homologically essential and as nearly one-to-one as possible. To accomplish this, we restrict to the case that Λ is *hyperbolic* (no eigenvalue has an algebraic conjugate on the unit circle) and *unimodular* (every eigenvalue of Λ is an algebraic unit).

There is a finitely generated $\mathbb{Z}$-module $GR \subset \mathbb{R}^n$ restricted to which Λ is a linear isomorphism. Let D denote the rank of GR and let A be a $D \times D$ integer matrix representing $\Lambda : GR \to GR$ in some basis. (A is hyperbolic.) There is then a rank D submodule of $H^1(\Omega_\Phi; \mathbb{Z})$, say $\langle \gamma_1, \ldots, \gamma_D \rangle$, invariant under Φ^*, restricted to which Φ^* is represented by the transpose of A. We proceed as follows. Each γ_i can be considered to be a (homotopy class of a) map $\gamma_i : \Omega_\Phi \to \mathbb{T}$, and their product yields $\Gamma : \Omega_\Phi \to \mathbb{T}^D$. We have $\Gamma \circ \Phi$ equals $F_A \circ \Gamma$ in cohomology (F_A being the hyperbolic toral automorphism induced by A). By lifting Γ to an appropriate abelian cover and applying a standard global shadowing procedure from hyperbolic dynamics, we homotope Γ to G.

We have shown that the $G : \Omega_\Phi \to \mathbb{T}^D$ so constructed is continuous and obeys $G \circ \Phi = F_A \circ G$. Furthermore, G is a.e. r-to-one for some $r \in \mathbb{N}$ and G is homologically essential in that $G^* : H^1(\mathbb{T}^D; \mathbb{Z}) \to H^1(\Omega_\Phi; \mathbb{Z})$ is injective.

Moreover, if in addition Λ is *Pisot family*, and the *generalized degree*, $D(\Lambda)$, of Λ equals the rank D of GR, then G is surjective and also semi-conjugates the $\mathbb{R}^n$-action on Ω_Φ with a Kronecker action on $\mathbb{T}^D$.

Thus the coordinate functions of G give D independent continuous eigenfunctions of the $\mathbb{R}^n$-action on Ω_Φ. Under these conditions, the eigenvalues of the $\mathbb{R}^n$-action are relatively dense in $\mathbb{R}^n$ and the tilings in Ω_Φ have the Meyer property. We conjecture the following: If Φ is a unimodular Pisot family substitution and $rank(H^1(\Omega_\Phi; \mathbb{Z})) = D(\Lambda)$ then the $\mathbb{R}^n$-action on Ω_Φ has pure discrete spectrum.

(Based on joint work with J.-M. Gambaudo, see [5]).

3.3 Fibonacci numbers and representations of quivers (Claus-Michael Ringel)

It is well-known that the entries of the dimension vectors of some distinguished 3-Kronecker modules are the Fibonacci numbers; the 3-Kronecker modules are triples of matrices with the same shape, thus representations M of the quiver Q with two vertices a, b and three arrows $a \to b$. Using covering theory, one may consider instead of Q its universal covering $\widetilde{Q}$, which is the 3-regular tree with bipartite orientation. Thus, instead of M, we now deal with a representations $\widetilde{M}$ of $\widetilde{Q}$, but this means that the two vector spaces given by M are written as direct sums of a large number of much smaller vector spaces M_i. In terms of dimensions, we exhibit in this way partition formulae for the Fibonacci numbers. The dimensions of the vector spaces M_i can be arranged to form two triangles, one for the even-index Fibonacci numbers, the other for the odd-index ones, and one may compare the triangles with the Pascal triangle of binomial coefficients. These distributions of numbers are additive functions on valued translation quivers, but also they may be constructed inductively by using some hook formula. The hook formula shows that the numbers along the inclined lines can be obtained by evaluating monic integral polynomials (but the actual coefficients of these polynomials are not known). One column of the first triangle has been identified by Hirschhorn (2008) as the number of Delannoy paths which do not horizontally cross the main diagonal. It seems astonishing that no other row or column had hitherto been recorded in Sloane's Encyclopedia of Integer Sequence.

There are intriguing relations between the two triangles: for example, differences along suitable arrows in one triangle are numbers which occur in the other triangle. Also, the left hand side and the right hand side of the odd-index triangle determine each other. All these results were found by looking at certain exact sequences involving Fibonacci modules, but they can be verified also recursively. There is another interpretation of the numbers in the triangles, namely as dimensions of some (subspace) representations of the 3-regular tree, now with a unique sink and no sources.

3.4 Stationary spatial stochastic processes and the inverse problem in pure point diffraction (Robert V. Moody)

The inverse problem in diffraction is the problem of recovering the physical distribution of a material from knowledge of its diffraction. The diffraction is a positive, centrally symmetric translation bounded measure in the Fourier dual space of the native space of the material. The question we raise ere is whether or not we can find solutions to this problem no matter what positive, centrally symmetric translation bounded measure we begin with.

The fundamental issue that arises in attempting to answer this question is what sort of mathematical object should we be looking for in trying to model the potential physical distribution of material whose diffraction is to be the given measure? In this paper we show that in the case of pure point diffraction we can always find solutions to this problem. These solutions come in the form of a new type of mathematical object which we call a stationary spatial stochastic process. The talk discussed the motivation for this concept out of ideas from stochastic point processes, and showed how it arises both as an extension of the Halmos-von Neumann theory of dynamical systems with pure point spectra and by a Gel'fand construction based on the eigenfunctions of the system.

At the end of the talk we discussed open problems around the explicit nature of the solutions created by the process, how the wealth of solutions to the problem may be filtered through the use of moments, and the apparent potential for some sort of cohomological extension to the theory.

The work is joint work with Daniel Lenz [12].

3.5 Generalised Thue-Morse systems (Uwe Grimm and Franz Gähler)

These two consecutive, closely related talks covered spectral and topological aspects of generalised Thue-Morse systems.

The first talk briefly summarised the proof of the purely singular continuous diffraction of the classical Thue-Morse sequence in the balanced weight case; see [3] and references therein. It then introduced generalised Thue-Morse substitutions generated by substitution rules $1 \to 1^k\bar{1}^\ell$, $\bar{1} \to \bar{1}^k 1^\ell$ on the two-letter alphabet $\{1, \bar{1}\}$, where $k, \ell \geq 1$ and $k = \ell = 1$ corresponds to the classical Thue-Morse case. All these rules give rise to purely singular diffraction measures in the balanced case. Their distribution functions possess uniformly converging Fourier series expansions with coefficients which are determined recursively, and the corresponding densities can be expressed as Riesz products. The pure point part of the dynamical spectra are recovered by factors which arise from the same sliding block map as in the classical case; the corresponding substitutions are generalisations of the period-doubling rule. The talk ended by showing how this approach generalises to bijective substitutions in higher dimensions, and explicitly considered the example of the squiral tiling. Again, it shows singular continuous spectrum, and a factor with maximal pure point spectrum can be constructed using a suitable block map.

In the second talk, topological invariants, in particular Cech cohomology groups, were computed for the whole series of generalised Thue-Morse and generalised period-doubling tiling spaces. For this purpose, each of the tiling spaces was constructed as an inverse limit using the Anderson-Putnam construction. A tiling space is approximated by a finite cell complex (the AP complex) in such a way that the inverse limit of the substitution acting on the AP complex is homeomorphic to the tiling space. As a consequence, the Cech cohomology is given by the direct limit of the substitution action on the Cech cohomology of the AP complex. The AP complexes could be chosen in such a way, that the sliding block map from the generalised Thue-Morse tilings to the generalised period-doubling tilings extends to the respective AP complexes, intertwining the substitution maps acting on them.

As a result, not only the cohomology of the respective tiling spaces is obtained, but also the embedding of the generalised period-doubling cohomology in the generalised Thue-Morse cohomology. All these computations could be carried out for the whole series of tiling spaces parametrised by the natural numbers k and ℓ. Using results recently derived by Greg Maloney (also presented at the workshop), the number of different AP complexes could be reduced to three for each of the generalised Thue-Morse and generalised period-doubling tiling spaces. The remaining dependence on k and ℓ is only in the substitution maps. For all choices of k and ℓ, the substitution acts with eigenvalues $k+\ell$, $k-\ell$ and -1 on the cohomology of generalised Thue-Morse tiling spaces, and with eigenvalues $k+\ell$ and -1 on the cohomology of the generalised period-doubling tiling spaces. From these results, also the dynamical zeta function for the substitution action on the continuous hull is readily derived.

(Based on joint work with Michael Baake).

3.6 Three aperiodic questions and their (lack of) progress (Aernout C.D. van Enter and Jacek Miękisz)

In this presentation, the following three questions were discussed, based on an ongoing collaboration between 1988 and 2000, and also further progress on them in so far as that occurred.
Question 1: Aperiodic order as order. How should one describe long-range order, and give spectral characterisations thereof?
Question 2: Where does aperiodic order come from? Can one find models of quasicrystals or 'weak crystals' in which either ground states or Gibbs states display aperiodic order?
Question 3: Aperiodic order as disorder. Can one compute and obtain interesting aperiodic examples of the Parisi overlap distribution (which was introduced for the paradigmatic disordered model, spin glasses)?

As for Question 1, in [11] the authors investigated the distinction between what is now called "diffraction versus dynamical spectrum", with an interpretation in terms of of atomic versus molecular long-range order. It became well-known afterwards, based on work by Baake, Lee, Lenz, Moody, Scholttmann and Solomyak, that pure point diffraction and pure point dynamical spectrum, under some mild assumptions, are equivalent properties of dynamical systems of translation bounded measures. But this type of equivalence does not extend to systems with continuous spectrum, as the example of the Thue-Morse sequences showed [11]. The diffraction spectrum of the Thue-Morse system is purely singular continuous, while the dynamical spectrum has a non-trivial pure point part in form of the dyadic rationals. This spectral information is not reflected in the diffraction spectrum.

However, this 'missing' part can be extracted from the diffraction of a factor, the so-called period doubling sequences, which are Toeplitz sequences. In [4], an even simpler example of this phenomenon is presented for a one-dimensional system of random dimers, which can be of $+-$ or $-+$ type, and which can be located on $2n, 2n+1$ or on $2n, 2n-1$ intervals. This system has absolutely continuous diffraction spectrum, but the long-range order associated to the location of the dimers provides an additional point in the dynamical spectrum. It thus appears that molecules can be more, but not less, ordered than their constituent atoms. A completely general statement to this effect is not yet available, however.

About Question 2, one can construct aperiodic tilings which are ground states for nearest-neighbor (tiling) models, or as aperiodic sequences, which are ground states for long-range interactions. Some stability and intrinsic frustration properties for tiling models have been proved, but as for positive temperatures (Gibbs states), one is still restricted to one-dimensional aperiodic long-range order, which occurs for infinite-range interactions. This can occur for one-dimensional long-range models, or for exponentially decaying interactions which are stabilised in two other directions; compare [14, 15]. To prove the existence of a quasicrystalline state for a short-range model remains open.

About Question 3, it was observed in [10] that continuous diffraction spectrum implies a trivial overlap distribution, whereas the Fibonacci sequences provide an example with a continuous overlap distribution and the period-doubling Toeplitz sequences have a discrete, ultrametric overlap distribution. Recently, in [9], this was extended to show that continuous overlap distributions occur for general Sturmian sequences (= 'balanced words' = 'most homogeneous configurations'). Moreover, for paperfolding sequences, a discrete ultrametric overlap distribution with dense support was found. Although in the theory of spin glasses a huge progress has occurred for mean-field models of the Sherrington-Kirkpatrick type (due especially to Guerra and Talagrand), not much is known about short-range models. Aperiodic examples may thus play a useful role in illustrating various possibilities. For instance, the fact that the overlap distribution is disorder-independent becomes much more plausible once one realises that one does not need disorder at all to obtain nontrivial overlap distributions. It would be interesting to obtain examples also in higher dimensions, via tiling constructions.

3.7 Random measures and diffraction (Matthias Birkner)

This talk elaborated an observation (due to Jean-Baptiste Gouéré) that connects the autocorrelation of a random measure with its so-called Palm distribution, a well-studied object in the fields of random measures and in stochastic geometry: Let Φ be a shift-ergodic signed random measure on $\mathbb{R}^d$ with locally square integrable total variation. Then, the natural autocorrelation $\lim_{n\to\infty} \frac{1}{\mathrm{vol}(B_n)} \Phi|_{B_n} * \widetilde{\Phi|_{B_n}}$ exists almost surely and is non-random (B_n denotes the ball of radius n around the origin and $\Phi|_{B_n}$ the restriction to that ball). It is given by the reduced second moment measure and can, in the case of a positive random measure, also be interpreted as the (scaled) intensity measure of the Palm distribution, Here, the latter has a natural interpretation as the configuration of Φ viewed 'from a typical point drawn from Φ'. The result was illustrated by explicitly computing the autocorrelation and the diffraction, its Fourier transform, for various cluster processes. These confirm the observation that additional randomness, coming from the independent clusters, modifies the diffraction of a given point process by adding an absolutely continuous component.

(This contribution is based on joint work with M. Baake and R. V. Moody [2]).

3.8 Dynamical methods in spectral theory of quasicrystals (Anton Gorodetski)

The Fibonacci Hamiltonian is a central model in the study of electronic properties of one-dimensional quasicrystals. It was shown by Süto that its spectrum is a zero-measure Cantor set for every non-zero value of the coupling constant. The question on the properties of the spectrum can be reduced to the question on dynamical properties of a so called trace map. In our joint work with David Damanik [7, 8], we studied the dynamical properties of the trace map and used them to describe the spectral properties of the Fibonacci Hamiltonian. In particular, we showed the following:

(i) For sufficiently small values of the coupling constant, the boundary points of a gap in the spectrum depend smoothly on the coupling constant. Moreover, the size of the gap tends to zero linearly as the coupling constant tend to zero;

(ii) For small values of the coupling constant, we have that the sum of the spectrum with itself is an interval. Therefore, the spectrum of the square Fibonacci Hamiltonian is an interval for small values of the coupling constant;

(iii) For small values of the coupling constant, the density of states measure of the Fibonacci Hamiltonian is exact-dimensional, the almost everywhere value of the local scaling exponent is a smooth function of the coupling constant, is strictly smaller than the Hausdorff dimension of the spectrum, and converges to one as coupling constant tends to zero.

3.9 On Proximality (Johannes Kellendonk)

Given a dynamical system (X, G, α) where X is a compact metric space, G a locally compact, σ-compact, Abelian group and α a minimal group action, we investigate the proximality relation $P \subset X \times X$. Two points $x, y \in X$ are *proximal* if $\inf_{t \in G} d(\alpha_t(x), \alpha_t(y)) = 0$, where d is the metric on X. We are in particularly interested in tiling or Delone dynamical systems, because the nature of the diffraction spectrum of the Delone set is tightly related to the spectral type of the dynamical spectrum of the system, and the latter can be studied with the help of the proximal relation, as will be developed.

The continuous eigenfunctions determine what is called the maximal equicontinuous (or Kronecker) factor of the dynamical system and the factor map π gives rise to an equivalence relation $R_\pi = \{(x, y) : \pi(x) = \pi(y)\}$ which contains P. The question is, how large are the typical equivalence classes of R_π, and in which way do they differ from the equivalence classes of P? This also leads to considering the minimal rank i.e. the smallest number of elements in an equivalence class of R_π and the set $Y \subset X/R_\pi$ of equivalence classes which contain only pairwise non-proximal points.

(Based on joint work with Marcy Barge [6]).

3.10 Measuring the complexity of tilings with infinite local complexity (Lorenzo Sadun)

A standard assumption in studying tilings is that there should only be a finite number of connected 2-tile patterns, up to translation. This is called Finite Local Complexity, or FLC. However, many interesting tilings have Infinite Local Complexity (ILC), either because there are infinitely many tile types, or because the tiles can slide past one another in a continuous manner. Examples include the pinwheel tiling, Toeplitz flows (which can model solenoids), and many fusion tilings.

Adapting a construction from the topological entropy of flows, we define a complexity function $C(\epsilon, L)$ at precision ϵ and length scale L. The important question is how this function behaves as $L \to \infty$ for fixed ϵ, and whether this behavior (e.g., bounded, or polynomial growth, or exponential with a particular exponent) is the same for all small ϵ. Such behavior is invariant under topological conjugacies. The behavior as $\epsilon \to 0$ for fixed L is *not* invariant, and is far less meaningful.

4 Scientific Progress Made

The main goal of the meeting was to bring people from the field of Aperiodic Order together and to exchange the recent advances, with some focus on spectral aspects. The field is developing rapidly, and expanding into a variety of directions. After several more specialized meeting (for instance on the topology of tiling spaces), this exchange was needed to keep track of the developments. We believe that this goal was fully reached.

Moreover, due to the different but related questions in neighbouring disciplines, it was a good opportunity to discuss with colleagues and start new collaborations. One notable instance emerged from the interaction between Aernout van Enter and two of the organisers (MB and DL), pointing a way to reach an equivalence result for dynamical versus diffraction spectrum beyond the pure point situation. Another instance is the realization that the work on tridiagonal matrices with Fibonacci diagonals and off-diagonals presented by William Yessen contains ideas that will be useful in a different context, namely orthogonal polynomials on the unit circle, where the obstacle of energy-dependence of a key quantity may be overcome by implementing those ideas in this context. This will be carried out in a collaboration between three of the workshop participants.

5 Outcome of the Meeting

The mathematical theory of aperiodic order was systematically started with the NATO workshop in 1995 and the ensuing long-term program at the Fields Institute, both organised by Robert V. Moody and Jiri Patera. The field has seen a steady development since then, and is likely to get some further push now by the Nobel Prize to Shechtman. This meeting was central in the sense that it showed how diverse the questions are, yet how well the different mathematical disciplines worked and work together to further our knowledge and understanding. It is fair to say that the interactive atmosphere of the meeting was outstanding, and that important directions for future research could be identified.

In summary, for a field like this, there is no alternative to an attractive meeting place such as BIRS or Oberwolfach, and we are confident that particularly this meeting initiated quite a number of high quality cooperations and publications.

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