FULL DESCRIPTION

1. Research Project Objectives

(scientific problem aimed to be solved by the proposed project, project's research hypotheses)

One of the fundamental problems of physics, the so-called crystal problem, is to understand causes of crystalline symmetry in low-temperature matter [1–7]. More precisely, why at sufficiently low temperatures and high pressure, atoms or molecules of macroscopic bodies tend to organize themselves to form periodic arrangements of perfect crystals? A fundamental law of statistical physics states that equilibrium behavior of systems of interacting particles results from the competition between energy and entropy of a system, that is the minimization of its free energy. At very low temperatures, the probability distribution on the set of particle space configurations is concentrated on those configurations with (almost) minimal energy since the entropy contribution to the free energy is negligible. At this point the basic question is: why should particle configurations with the minimal interaction energy necessarily be periodic or exhibit at least some sort of long-range order or, in other words, why will configurations minimizing energy functionals of translation-invariant interactions break that symmetry? A typical example is the phase transition at the freezing temperature of water, where liquid water with a full translational and rotational symmetry turns into ice crystals which break those symmetries.

It was traditionally accepted that realistic physical interactions force particles to form periodic arrays. However, this was never proved; rather, it was an axiom of solid state physics. This situation changed dramatically with the discovery of quasicrystals by Dan Shechtman in 1982 [8]. He showed that a certain alloy exhibits five-fold rotational symmetry which cannot appear in periodic arrangements of atoms. So the old question became rephrased: how to deduce aperiodic long range-order (crystalline, quasi-crystalline or else) from translation-invariant interactions between particles? A natural first specific problem is to construct models of interacting particles such that only non-periodic particle configurations (called ground-state configurations) minimize the energy. A follow-up problem is then to show that such configurations are stable in an appropriate sense. Here stability refers to two different aspects: first, we need that small perturbations of interactions (which in reality are inevitable) do not change ground-state configurations (zero-temperature stability) and, second, that non-periodic ground-state configurations are stable against thermal fluctuations (low-temperature stability), in the sense that they typically change only by a small amount, that is, on sets of low density. Such stability questions are the leitmotif of this grant proposal.

We will focus on lattice-gas models of interacting particles. In such models every site of an infinite regular square or cubic lattice is occupied by at most one particle. We assume that there is a finite number of particle types and that particles located at lattice sites interact through nearest-neighbor or longer range translation-invariant interactions. It is worth emphasizing here that the underlying lattice is periodic; the objects of our interest are non-periodic particle configurations (i.e., assignments of particle types to lattice sites). We are interested in examples of interactions for which only non-periodic configurations minimize energy of the system, that is all ground-state configurations are non-periodic (the precise definition of a ground-state configuration will be provided later). At non-zero temperatures, to minimize the free energy of a system one constructs Gibbs measures (called grand-canonical ensembles by physicists or simply Gibbs states) on the space of all particle configurations (with an appropriate σ-algebra of measurable sets). There is a natural action of lattice translations on measures and therefore one can define non-periodic measures. Now we can state precisely the main open problem we would like to address.

Main Open Problem: Does there exist a translation-invariant finite-range interaction on a regular lattice for which there exists a non-periodic Gibbs measure at all sufficiently low temperatures?

The answer to this problem may depend on the dimension of the lattice. There is a long standing conjecture that any two-dimensional lattice-gas model with finite-range interactions and a finite number of particle types has only a finite number of extremal Gibbs states. A construction of a three-dimensional model with the desired property thus seems more plausible. We should notice here the possible relevance of the work of Peter Gács who claims to construct an infinite number of stationary measures in a certain one-dimensional cellular automaton [9–11]. The connection between stationary measures of one-dimensional cellular automata and Gibbs states on space-time trajectories was presented in [12]. We will explore this connection in one of our research tasks.

Some of our models are based on non-periodic tilings which brings us back in time to one of David Hilbert's problems posed in 1900. The second part of his 18-th problem can be stated in the following way: Does there exist a polygon which can tile the plane but only in a non-periodic way? In any tiling, all points of the plane are covered and tiles do not overlap except their boundaries. A more modest version of this problem was put forward by Hao Wang in 1961 [13] in the context of decidability in computer science. He asked if there exists a finite number of prototiles — squares with notches and dents (sometimes called dominoes) — that can be used to tile the plane so that all tilings are non-periodic. The tilings necessarily arrange in the form of the square lattice with notches and dents of adjacent tiles forced to fit together by suitable matching rules. Wang's question was answered affirmatively by Robert Berger in 1966 [14]. Berger's example uses over 20 thousand prototiles; this was improved in 1971 by Raphael Robinson's example of 56 prototiles [15]. The number of prototiles which cover the plane but only in a non-periodic way was further brought down by many people; the last most recent construction involves only 11 prototiles [16].

In the mean time, Roger Penrose addressed the Hilbert problem and found tiles — the now famous kite and dart — that can be used to cover the plane but only in a non-periodic fashion [17]. Accidentally, the diffraction pattern associated with Penrose's tilings has a five-fold symmetry (which is forbidden in translation-invariant crystals) just as the one observed several years later in Shechtman's work. It is also worth noting that just before the publication of the discovery of quasicrystals, in his influential book [4], Nobel laureate Philip Anderson offered a "mathematical" proof that every translation-invariant interaction should have periodic ground-state configurations. This illustrates why it is important to study mathematical models of quasicrystals. Indeed, mathematics gives proper tools to deal with infinities that are present here in a natural way in the concept of non-periodicity.

One of the leading themes of this grant proposal is an investigation of the rigidity of non-periodic tilings. We use examples of a finite family of prototiles that tile the plane only in a non-periodic way and construct examples of lattice-gas models with translation-invariant nearest-neighbor (or next nearest-neighbor) interactions that do not possess any periodic ground-state configurations. Our general approach is as follows: first we identify different prototiles with types of particles, then we translate matching rules into interactions by assigning positive energy, say 1, to any pair of mismatched tiles while giving energy zero to all pairs of matching tiles. The resulting lattice-gas model has only non-periodic ground-state configurations corresponding to non-periodic tilings. The rigidity of tilings can be then seen as zero and low-temperature stability of corresponding classical-lattice gas models.

On our way towards the main aim of our project we will investigate various mathematical properties of non-periodic tilings and non-periodic structures in general. We will often work in the general framework of symbolic dynamical systems. In all of our models, all ground-state configurations (or just configurations of interest) are non-periodic. Notwithstanding, there is a unique translation-invariant probability measure, also called a ground state, that is supported by the closure of the orbit under action of translations of any chosen configuration. We remark that non-periodicity does in no way mean disorder. There are in fact many ways to quantify order in non-periodic structures such as almost periodicity, non-mixing of ground-state measures, etc and one may also define some other types of order depending on the context. The basic question we will address here is if some kind of order survives at non-zero temperatures.

The non-periodic ground-state measure is uniquely ergodic in the sense that any local pattern appears with the same frequency in all configurations. However, a more quantitative version of this limit statement seems to be needed in order to control low-temperature stability of non-periodic ground states. One such version, the strict boundary condition, was formulated in [18]. It roughly states that in any finite region, the number of occurrences of any finite pattern differs from the product of its frequency and the volume (area) of the region by the contribution proportional to the boundary of the volume (for definitions see Section 4). It is our hypothesis that such a property forms a necessary and sufficient condition for low-temperature stability of non-periodic ground states.

We will investigate overlap distributions [19] of non-periodic measures of uniquely ergodic systems and their connections with spectral properties of such measures. Both overlap distributions and the spectrum (either the spectrum of the translation operator in an appropriate L^2 space or a Fourier transform of a correlation function; see [20]) might be signatures of non-periodic order [21–24].

We will also study substitution dynamical systems, where non-periodic sequences on a one-dimensional lattice are generated by substitution rules, Fibonacci or Thue-Morse for example [25]. Tiling dynamical systems are examples of systems of finite type in which uniquely ergodic measures, and thus also the configurations in their support, are completely characterized by the absence of a certain family of finite patterns. One can prove that there are no one-dimensional non-periodic systems of finite type [26]. However one can try to find minimal sets of forbidden patterns which characterize such systems. It is one of our goals to find such minimal sets for various classes of substitution dynamical systems; an example of such a construction for the Thue-Morse substitution rule was provided in [27]. Any system of finite type can be seen as a classical lattice-gas model with finite-range interactions assigning positive energy to forbidden patterns (as was showed in [28], the reverse correspondence is not always possible). In an analogous way, given a minimal set of forbidden patterns one can easily construct one-dimensional Hamiltonians whose unique non-periodic ground state is exactly the (implicit) uniquely ergodic measure avoiding the forbidden patterns. One of our goals will be to see whether extending such one-dimensional models by ferromagnetic Ising-type interactions in (at least) two other spatial directions — the so called stacking — produces non-periodic Gibbs measures that are only small perturbations of the original uniquely ergodic measures. It is worth to mention here that some substitution systems can be represented by appropriately constructed two-dimensional tilings [29].

To motivate a final class of questions, we would like to mention numerical results [30–33] indicating phase transitions in classical lattice-gas models without periodic ground states. Here new "aperiodic-order-sensitive" observables were introduced that vanish at high-temperatures for which Monte-Carlo simulations showed (e.g., by analyzing suitable overlap distributions [30]) non-zero value at low temperatures. While the existence of non-periodic Gibbs states is not necessarily claimed there, the existence of some sort of phase transition is quite apparent. We will check how the possible existence of non-periodic Gibbs states is consistent with results of the above mentioned papers.

The present project has a strong interdisciplinary flavor drawing ideas from statistical physics, ergodic theory, substitution and tiling systems, and computer science. The principal goal is to develop rigorous understanding of fundamental questions about the origins of aperiodic long-range order in physical systems and to explore mathematical structures that are relevant for breaking of translation invariance due to collective effects in physical materials.

2. Significance of the project

(state of the art, justification for tackling specific scientific problems by the proposed project, pioneering nature of the project, the impact of the project results on the development of the research field and scientific discipline, economic and societal impact)

Mathematical investigations of non-periodic structures have been conducted for a long time. These efforts intensified after the discovery of quasicrystals. Indeed, several branches of mathematics were provided with new motivations and problems to be tackled. Various constructions of non-periodic structures were no longer just abstract toy models and it begun to be obvious that careful mathematical study of the these constructions might provide new insights into physics of real materials, the quasicrystals.

The first classical lattice-gas model without periodic ground state-configurations was constructed by Charles Radin in [34]. A series of papers by Radin and the author of this proposal followed dealing with stability properties of such models. It was proven that generically (in the sense of the Baire category) lattice-gas models with long-range interactions do not have periodic ground-state configurations, yet, on the other hand, generically ground-state measures are not mixing [35, 36]. Lack of mixing may be interpreted as the presence of long-range order. In [37] we constructed a model with a unique translation-invariant ground-state configuration which is not stable at any low temperature. That served, in fact, as a counterexample to a hypothesis due to Dobrushin and Shlosman [38]. The presence of non-periodic ground-state configurations corresponding to Robinson's tilings was essential in the construction of a counterexample. The best result for finite-range interactions known up till now is the construction of a model with an infinite sequence of phase transitions of Gibbs states with period-doubling at an infinite sequence of critical temperatures [39], see also [40]. Unfortunately this sequence of temperatures converges to zero so the true non-periodic order is present only at zero temperature. Recently an analogous result has been shown in the physics literature [41].

It was shown in [42] that any uniquely ergodic measure can be seen as a ground-state measure of some long-range arbitrarily many-body interaction — again, assigning positive energy to patterns (decaying sufficiently fast to zero with the size of the patterns) which have zero frequencies in the given ergodic measure. The other extreme are systems (subshifts) of finite type which are characterized by the absence of finite number of finite patterns. Then uniquely ergodic measures are ground-state measures of finite-range interactions. We showed in [28] that the class of uniquely ergodic ground-state measures of finite-range interactions in lattice-gas models is larger than the class of uniquely ergodic measures of subshifts of finite type. In other words, there are ground-state measures which minimize the energy functional of finite-range interactions that cannot be uniquely characterized by the absence of any finite set of patterns.

W. H. Gottschalk and G. A. Hedlund proved in 1964 [43] that Thue-Morse sequences of two symbols are uniquely characterized by the absence of blocks BBb, where B is any block of symbols and b is the first symbol of the block B. We proved in [27] that to characterize Thue-Morse sequences it is enough to forbid patterns consisting of four symbols only. Then we showed that the uniquely ergodic Thue-Morse measure i s the unique ground-state measure of the one-dimensional Ising model with exponentially-decaying four-spin interactions. As one of our research tasks, we would like to find minimal sets in the sense of minimizing the number of symbols in forbidden patterns which characterize other substitution dynamical systems. That would enable us to construct one-dimensional Hamiltonians with non-periodic ground-state measures and then to investigate low-temperature stability of such measures.

In [18] we formulated the so-called strict boundary conditions that characterize (as already noted above) the speed of convergence of empirical density of finite patterns to their infinite-volume limit; precise definitions will be given in Section 4. We also proved that these are necessary and sufficient conditions for zero-temperature stability of ground states. Non-periodic ground-state configurations of lattice-gas models based on Robinson's tilings do not satisfy the strict boundary conditions even for one-site patterns; i.e., the density of particle types. In [44] we proved that the ground-state configurations of a lattice gas-model based on Robinson's non-periodic tilings are unstable with respect to the addition of a chemical potential. One of the goals of this grant project is to check if the strict boundary conditions are necessary and sufficient conditions for low-temperature stability of non-periodic ground states. So far, we do not know of any examples of non-periodic ground states that satisfy the strict boundary conditions. Recently, there have been some examples of non-periodic structures with such properties [45]. However it is not known if they result from some local matching rules. To investigate the possibility of such a formulation is one of the goals of this project. There also appeared some new constructions of aperiodic tilings for which their authors claims some sort of rigidity [46–48]. We will plan to examine if this rigidity helps to establish zero and low-temperature stability.

In one-dimensional long-range Hamiltonians one can force non-periodicity by methods not providing control over the tail of an interaction. In [49] we constructed a non-periodic low-temperature Gibbs measure in a lattice-gas model with summable interactions having Thue-Morse ground-state configurations. It was the first example of such a measure and the first microscopic model of a quasicrystal, see also [50]. The construction is based on identifying Gibbs measures and tangent functionals, and using a convex-analysis argument. For exponentially decaying interactions which are extended in two other spatial dimensions by ferromagnetic interactions we used cluster expansions to construct non-periodic Gibbs measures [51]. The two above approaches are quite abstract; in particular, they do not produce non-periodic Gibbs measures for the original Thue-Morse interactions introduced in [27].

In probabilistic cellular automata, lattice-gas configurations evolve in discrete moments of time. The probability of having a particular particle at a particular lattice site at time t depends on the states of neighboring sites at time $t-1$. A basic problem in probabilistic cellular automata is to describe their stationary states in the infinite-volume limit. There is a correspondence between stationary states of d-dimensional cellular automata and Gibbs states on $d+1$ dimensional space-time configurations (stationary states are space projections of Gibbs states) [12]. There was a long standing hypothesis (the so called positive-rate conjecture) in one-dimensional cellular automata, that if all transition probabilities are positive, then there is a unique stationary state. The conjecture was refuted by Peter Gács [9–11] who constructed a one-dimensional cellular automaton with (at least) two stationary states. In such a non-ergodic system, the initial conditions are "remembered." In a subsequent work, Gács [10] claims a construction of an automaton in which in a certain sense any initial condition is remembered. This would give rise to an infinitely (uncountably) many extremal Gibbs states, some of them being non-periodic. Thanks to the above identification, this would provide a counterexample to the hypothesis that in two-dimensional models there are always finite number of extremal Gibbs states. In particular, cellular automata may give us another way of constructing non-periodic Gibbs states.

In our research project we address several hypotheses which concern non-periodic structures. They are connected with the fundamental question: How does global (non-periodic) order arise from local rules? Stability of non-periodic configurations will make possible constructions of machines (in a computer-science sense) which are tolerant to errors and noise.

3. Work plan

(outline of the work plan, critical paths, state of preliminary and initial research indicating feasibility of research objectives)

In our project we will plan to address the fundamental problem of the existence of non-periodic Gibbs measures in classical lattice-gas models with short-range interactions. We plan to explore certain paths towards our main goal with clear checkpoints. As a guiding framework we will use the strict boundary conditions; we will analyze to what extent they form sufficient and necessary conditions for stability of non-periodic ground states.

We begin by calculating spectral measures and overlap distributions for certain substitution as well as tiling systems. Both the spectrum and the overlaps may be seen as signatures of non-periodic order. We will investigate relations between these two objects. For example, in the so-called paper-folding system, the spectral measure equals the overlap distribution [52]. Are there other systems with that property? A fundamental question is: Do results obtained for abstract non-periodic structures still hold if we restrict ourselves to structures which are ground states for certain short-range interactions? Do they hold for generic interactions in certain spaces? Here we will follow the ideas presented in references [35, 36].

A special attention will be given to the so called most-homogeneous sequences (known also as Sturmian or balanced systems) [53]. These are the ground-state configurations of infinite-range convex repelling interactions between particles additionally subject to a chemical potential [53–55]. The competition between repelling pair interactions and the chemical potential favoring the presence of particles produces ground-state configurations with all possible particle densities, including irrational ones. Ground states as function of chemical potential form a Cantor set also known as the Devil's staircase. Two-dimensional analogues of most-homogeneous configurations realized as ground states of a finite-range lattice-gas model were presented in [28]. Properties of such two-dimensional models were discussed in physics literature in [56].

As another direction of effort, we will explore the existence of stratified non-periodic Gibbs measures in lattice gas-models with one-dimensional interactions having as ground-state configurations most-homogeneous configurations and other non-periodic structures. The idea behind this is as follows. We extend a one-dimensional system in two other spatial dimensions by ferromagnetic Ising-type interactions. In the absence of one-dimensional interactions we have uncoupled Ising models. Below the Curie temperature, these models exhibit magnetic order; in each plane there are two two-dimensional extremal Gibbs measures with up and down magnetization. In particular, the uncoupled system possesses uncountably many Gibbs measures corresponding to all double-sided sequences of pluses and minuses. Now we would like to enforce by energy our non-periodic structure by an appropriate one-dimensional interaction. But we should not forget about entropy. As a conceptual starting point one can take interactions corresponding to Thue-Morse systems [27]. Unfortunately, the Thue-Morse sequences do not satisfy strict boundary conditions and, as we have shown in [49], a simple 4-body interaction based on the minimal set of forbidden patterns extended in two other directions by ferromagnetic Ising-type interactions does not produce non-periodic Gibbs states. The reason is that there are periodic configurations which have more low-energy excitations than the Thue-Morse sequences such that the entropy contribution to the free energy is larger than the energy cost. This shows why it is important to look for non-periodic structures satisfying the strict boundary conditions.

The above discussion leads us in a natural way to models with finite-range interactions. To follow the above idea we have to construct four-dimensional models. But first we have to look for tiling that satisfies the strict boundary conditions. Some encouraging results have recently been presented in [45]. The author constructed some structures with the strict boundary property. We will examine thoroughly this construction to see if these structures can be forced by some local matching rules. There appeared recently some other constructions of non-periodic systems with new interesting properties [46–48]. We will examine whether such properties are relevant to zero and low-temperature stability.

The construction presented in [48] is based on Kleene's fixed-point theorem. It is worth mentioning that similar ideas were used by Peter Gács in his construction of cellular automata violating the positive-rate conjecture [9–11]. We will explore connections between non-periodic tilings and error correcting automata of Gács. We plan to address a general question of stability of non-periodic structures in the framework of non-equilibrium statistical mechanics. We would like to see whether the dynamic character of systems helps to stabilize non-periodic structures.

Research tasks:

1. **Spectral measures and overlap distributions**

   Computation of spectral measures and probability distributions of the overlaps of one-dimensional substitution and other non-periodic systems, Sturmian systems in particular, and also of some two-dimensional tiling systems.

   Generic dynamical systems are weak mixing but not mixing [57, 58] and generic operators have singular spectrum (Simon's wonderland theorem [59]). We hope to check if the same holds for ground states in an appropriate sense.

Let the diffraction spectrum not contain an absolutely continuous part. We would like to prove that the same holds for the dynamical spectrum. Note that this statement, without the "absolutely", was proven in [23].

Characterization of systems for which the spectral measure equals to the overlap distribution. This property is known to hold for paperfolding sequences. Mendès-France has raised the question, in how much generality this is true [52].

2. **Stratified Gibbs measures of fast-decaying interactions**

   Construction of Hamiltonians based on one-dimensional non-periodic structures with minimal sets of forbidden patterns. We extend such Hamiltonians by ferromagnetic Ising-type interactions in two other spatial dimensions. Constructing Gibbs measures for such three-dimensional Hamiltonians. Looking for sufficient conditions for the existence of non-periodic Gibbs measures for such Hamiltonians.

3. **Non-periodic Gibbs measures of finite-range interactions**

   Construction of Gibbs measures for finite-range interactions based on recent examples of non-periodic tilings. Proving the existence of non-periodic Gibbs measures for abstract systems satisfying strict boundary property. Construction of tiling systems with strict-boundary property.

4. **Gibbs measures in probabilistic cellular automata**

   Given a tile set, we ask whether there is a (deterministic) cellular automaton that ”washes out” finite islands of errors (as in Toom's cellular automata [60]) from any valid tiling. An argument of Gács would ensure then the recovery from sufficiently weak Bernoulli noise: starting with a valid tiling modified at the points of a low-density Bernoulli set, the CA converges to the set of valid tilings. We would like to get stability even if there is noise at each step (in the sense of Toom's CA) hence getting some sort of 3-dimensionl quasicrystal.

   We will check usefulness of the Gács construction in [10] in constructing 2-dimensional quasicrystals.

   We will study models of stacked cellular automata (as presented in [61]) in the context of non-periodic Gibbs states.

4. Research Methodology

(underlying scientific methodology, data reduction and treatment schemes, type and degree of access to the equipment to be used in the proposed research)

Classical lattice-gas models

All our research tasks concern discrete models. We investigate properties of non-periodic arrangements of symbols or particles to regular lattice sites. We construct minimal Hamiltonians for which such arrangements are ground-state configurations which minimize the energy of interacting particles. We work in the framework of classical (non-quantum) lattice gas-models. To deal with non-periodicity one has to consider infinite systems. Now we introduce formally lattice-gas models of interacting particles.

In classical lattice-gas models every site of $\mathbb{Z}^d$, $d \geq 1$ is occupied by one particle. There are n types of particles. $\Omega = \{1,...,n\}^{\mathbb{Z}^d}$ is the set of all particle configurations. For a finite subset $\Lambda \subset \mathbb{Z}^d$, $\Omega_\Lambda = \{1,...,n\}^\Lambda$.

Interaction potential Φ is a family of functions indexed by finite subsets Λ

$$\Phi = \{\Phi_\Lambda\}_{\Lambda \subset \mathbb{Z}^d}; \;\; \Phi_\Lambda : \Omega_\Lambda \to \mathbb{R}.$$

Φ is a **potential of a finite range** r if $\Phi_\Lambda \equiv 0$ for $\mathrm{diam}(\Lambda) > r$.

Φ is **a translation-invariant potential** if $\Phi_{\Lambda+a}(\tau_a X) = \Phi_\Lambda(X)$
for every $a \in \mathbb{Z}^d$, where τ_a is translation by vector a that is $(\tau_a X)_i = X_{i-a}$.

a Hamiltonian in a finite volume Λ is a function $H^\Phi_\Lambda = \sum_{V \subset \Lambda} \Phi_V$.

$Y \in \Omega$ is a **local excitation** of $X \in \Omega$, $X \sim Y$ if $|\{i \in \mathbb{Z}^d : Y_i \neq X_i\}| < \infty$.

For $Y \sim X$, **a relative Hamiltonian** is defined as
$H^{\Phi}(Y|X) = \sum_{\Lambda \subset \mathbb{Z}^d} (\Phi_\Lambda(Y) - \Phi_\Lambda(X))$.

A basic notion in the statistical physics of interacting particles is the notion of a ground-state configuration. Intuitively it is a configuration of the minimal energy. However, as we have already written, we have to consider infinite systems and usually the energy of an infinite configuration is infinite. We might then consider the energy density.

$$e(X) = \liminf_{\Lambda \to \mathbb{Z}^d} \frac{H^{\Phi}_{\Lambda}(X)}{|\Lambda|}$$

is **the energy density** of configuration $X \in \Omega$.
We would like to define ground-state configurations as those having minimal energy density. Let us notice however that if X is a ground-state configuration then any local excitation has the same energy density so it would be also a ground-state configuration which obviously is absurd. To avoid the above problems we define ground-state configurations in the following way.
$X \in \Omega$ is a **ground-state configuration** for potential Φ
if for every local excitation, $Y \sim X$, $H^{\Phi}(Y|X) \geq 0$.

One can prove that every translation-invariant finite-range interaction has at least one ground-state configuration. It may happen however that none of them are periodic. Anyway ground-state configurations minimize the energy density.

In the project we will study systems without periodic ground-state configurations or generally systems without periodic configurations but with a unique translation-invariant probability measure supported by them.
Let $\delta_{\tau_a X}$ is a measure assigning 1 to the configuration $\tau_a X$ and $X \in \Omega$ is a ground-state configuration.

$$\frac{1}{|\Lambda|} \sum_{a \in \Lambda} \tau_a X \to \mu \;\; as \;\; \Lambda \to \mathbb{Z}^d$$

In other words, there is a unique translation-invariant measure supported by the closure of the orbit $\{\tau_a X; a \in \mathbb{Z}^d\}$.

In other words, let X be any ground-state configuration in the support of μ and let ar any local arrangement of particles, n_{ar} is the number of appearances of ar in X in a box of size L centered at $a \in \mathbb{Z}^d$. Then

$$\frac{n_{ar}}{L^d} \to w_{ar} \;\; uniformly \;\; in \;\; a \in \mathbb{Z}^d$$

Such μ is called uniquely ergodic.

Substitution dynamical systems

Thue-Morse double-sided sequence of two symbols, 0 and 1 (a configuration on $\mathbb{Z}$), is generated by the following substitution,

$0 \to 01$

$1 \to 10$

Let μ_{TM} be the uniquely ergodic measure supported by the closure of the orbit of the above Thue-Morse sequence generated by the above rule [25]. It was proved in [43] that all sequences in the support of μ_{TM} are uniquely characterized by the absence of patterns BBb, where B is any sequence of 0's and 1's, and b is its first symbol. We proved in [27] that Thue-Morse sequences are also uniquely characterized by the absence of 4-site patterns

$b...b........b...b, \;\; b = 0, 1,$

where b's within pairs are at a distance 2^r and pairs are at a distance $(2p+1)2^r$, $r, p \geq 0$.

It allowed us to construct an exponentially decaying 4-spin Hamiltonian with the Thue-Morse measure μ_{TM} as its unique ground state. We would like to find minimal sets of forbidden patterns for other substitution dynamical systems and for Sturmian (most-homogeneous) systems.

Strict boundary conditions

Let H be a two-dimensional finite-range non-frustrated Hamiltonian (for example based on non-periodic tilings) with a uniquely ergodic ground-state measure. The absence of frustration means that all interactions can be minimized simultaneously.
For $Y \in \Omega$, $B(Y)$ is the set of broken bonds of Y that is $B(Y) = \{\Lambda, \Phi_\Lambda(Y) > min_Z \Phi_\Lambda(Z)\}$

$X(A)$ is a local ground-state configuration on a finite set of lattice sites A if it does not have broken bonds in A. Let us emphasize that such configuration may not be extendable to an infinite ground-state configuration.

Condition 1: The lattice-gas model satisfies the strict boundary condition for all local ground-state configurations and a local arrangement ar if for some C_{ar}

$$|n_{ar}(X(A)) - \omega_{ar}|A|| < C_{ar} P(A),$$

where ω_{ar} is the frequency of ar in the ground-state measure, $n_{ar}(X(A))$ the number of ar appearances in $X(A)$, $|A|$ is the number of lattice sites in A, and $P(A)$ is the length of the boundary of A.

Now let X be a ground state-configuration and $Y \sim X$, $n_{ar}(Y|X)$ the difference of the number of ar appearances in Y and X.

Condition 2: The lattice gas-model satisfies the strict boundary condition for local excitations and an arrangement ar if there exists C_{ar} such that for any ground-state configuration X and $Y \sim X$,

$$|n_{ar}(Y|X)| < C_{ar} B(Y).$$

We have proven in [18] that Condition 1 and Condition 2 are equivalent and that a uniquely ergodic ground-state measure of non-frustrated Hamiltonian is stable against perturbations of range r if and only if the above strict boundary conditions are satisfied for arrangements of range r.

Open Problem: Construct a non-frustrated classical lattice-gas model with a finite-range interactions and with a uniquely ergodic non-periodic ground-state measure which satisfies strict boundary conditions for all finite arrangements of particles.

Spectral measures and overlap distributions

We will use spin language here. At every site i of the one-dimensional lattice Z there is a spin variable σ_i which can attain the values $\pm$. An infinite lattice configuration is an assignment of spin orientations to lattice sites, that is an element of $\Omega = \{-1,1\}^Z$. We will consider uniquely ergodic measures on Ω. The support of such measures can be realized by appropriate substitution systems, tiling systems or in particular ground-state measures of certain Hamiltonians. There are many ways to describe positional long-range order in noncrystalline structures such as quasicrystals. Two main approaches involve spectral properties. One can consider the spectrum of translations acting as unitary operators on an appropriate Hilbert space, the so-called dynamical spectrum. In our case it is $L^2(\mu)$, where μ is a uniquely ergodic measure. To be precise we look for a spectrum of a shift operator T on $L^2(\mu)$, where $Tf(i) = f(T(i))$ for a function $f \in L^2(\mu)$. Let $C_f(n) = \mu(fT^n)$ By Bochner's theorem one can write $C_f(n) = \int_0^{2\pi} exp(i2\pi\lambda n) m_f(d\lambda)$, where m_f are measures on the interval $[0,2\pi]$. If for any choice of f, m_f has a pure point, singular continuous, or absolutely continuous part in its Lebesgue decomposition we say that the spectrum of the shift has a pure point, singular continuous, or absolutely continuous component, respectively. If the point spectrum consists solely of finitely many points, one interprets this as a crystal; if one has a dense point spectrum, one has a quasicrystal. In the second approach one considers the diffraction spectrum of atoms placed at lattice sites, that is one takes $f = f(0)$ in spectral measure. Dynamical and diffraction spectra in many examples were discussed in [20–23], see also [24] and references therein.

Another characterization of order is given by overlap distributions. Let X and Y be configurations in the support of μ. The overlap of X and Y is defined by

$$q_{XY} = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \sigma_i(X) \sigma_i(Y).$$

The Parisi overlap distribution $p(q)$ is the distribution of q_{XY} with respect to the product measure $\mu \otimes \mu$. It is known that weakly mixing measures have continuous dynamical spectrum. It is easy to see that such measures have an overlap distribution concentrated at $[\mu(\sigma_0)]^2$. We will study relations between dynamical spectra, diffraction spectra, and overlap distributions in the context of order in non-periodic structures. We would like to emphasize that our investigations go beyond traditional ergodic theory - all concepts, relations and theorems are considered for ergodic measures which are ground states of certain Hamiltonians.

Gibbs measures

Let $X \in \Omega$ be one of the non-periodic ground-state configurations of Hamiltonian H and Λ_L be the square of size L centered at the origin.

$$\Omega^X_{\Lambda_L} = \{Y \in \Omega, Y(\Lambda^c_L) = X(\Lambda^c_L)\}$$

$$\rho^X_{T,\Lambda_L}(Y) = \frac{e^{-\frac{H(Y|X)}{T}}}{\sum_{Z \in \Omega^X_{\Lambda_L}} e^{-\frac{H(Z|X)}{T}}}$$

is a finite-volume Gibbs measure, T is the temperature of the system.

One can show the existence of the thermodynamic limit (with the weak* convergence of measures),

$$\rho^X_{T,\Lambda_L} \to^{L \to \infty} \rho^X_T$$

We would like to prove that

$$\rho^X_T(Y \in \Omega, Y(0) \neq X(0)) > 1 - \varepsilon(T)$$

$$\varepsilon(T) \to 0 \ \ as \ \ T \to 0.$$

ρ^X_T would be then a non-periodic Gibbs state, a small perturbation of non-periodic ground-state configuration X. To achieve such a goal we plan to use Pirogov-Sinai cluster expansions [62, 63] in various models with non-periodic ground states.

Classical lattice-gas models based on non-periodic tilings

Our starting point is a non-periodic tiling of the plane. As an example of our construction we will use here Robinson' tilings [15]. He designed 56 square-like tiles (Wang tiles or dominoes) - squares with notches and dents on their sides. He proved that such tiles can tile the infinite plane but only in a non-periodic way. In any tiling, centers of tiles form the square lattice and notches and dents of adjacent tiles match. One can show that there is a unique translation-invariant probability measure supported by all such tilings, the support is the closure (in an appropriate topology) of the translation orbit of any tiling. We construct a classical lattice-gas model in the following way. We identify different tiles with types of particles. If two tiles do not match then the interaction energy between corresponding particles is positive, say 1, if they match then the energy is 0. It is easy to see that any tiling gives rise to a ground-state configuration with the zero interaction energy. Such a classical lattice-gas model (with nearest and next nearest-neighbor interactions) has only non-periodic ground-state configurations and a unique ergodic translation-invariant ground-state measure. The model does not satisfy the strict-boundary condition and it follows the ground state is unstable both at zero [44] and positive temperatures [39]. Our goal is to look at other non-periodic tilings. In this context especially interesting is a recent construction in [48]. This new tiling has two properties which might be useful in proving zero and low-temperature stability. The first property called strong aperiodicity ($\alpha - aperiodicity$) indicates that any tiling is far from any periodic tiling. More precisely

$X \in \Omega$ is α-aperiodic if for every $a \in \mathbb{Z}^2$ there exists N such that in every square whose side is at least N, the fraction of sites i such that $X_i \neq X_{i+a}$ exceeds α.

It is easy to see that Robinson's tilings are 0-aperiodic. The second property, resistance to sparse errors, says that one can erase certain mistakes (non-matching tiles) and the created hole can be tiled giving rise to an infinite-tiling. We will check if such a property is related to strict-boundary conditions and can it be used to prove low-temperature stability of the corresponding ground-state measure. Moreover, the autors of [48] write that their construction "is flexible enough to achieve some additional properties of the tile set" We will explore this possibility to construct tile sets with properties essential for low-temperature stability.

5. International collaboration

(significance of the project for international collaboration, benefits of international cooperation, value added of collaboration with foreign partner(s), scope of cooperation)

The leading foreign partner of this project is Aernout van Enter. We have worked together for many years on mathematical models of quasicrystals, we published together 8 papers, our results are discussed in this proposal. Then for several years I was not working on this subject. Unexpectedly in 2011 I was invited to a workshop in BIRS center in Canada to make a presentation of old open problems in mathematical quasicrystals. It appeared that these problems are still unsolved. Moreover, some people in the workshop get interested to get back to them. Then I was asked to co-organize ICQ12, 12th International Conference on Quasicrystals in Kraków in 2013. I was a chairman of the mathematical session and again I learned the state of the art of quasicrystal research. Finally I was invited in May 2016 to the workshop in Lorentz Center in Leiden to make an introductory talk on quasicrystal problems. During these three meetings I discussed new ideas with Aernout van Enter. We made a list of important research problems to tackle. With the second foreign partner, Marek Biskup, I worked many years ago on the construction of non-periodic Gibbs states in finite-range classical lattice-gas models, however without a success. I was visiting Marek Biskup at UCLA a year ago and we started to work again on the main problem of quasicrystals. In meantime there appeared new tiling systems with new properties which might be helpful in our constructions. Marek Biskup is a probabilist, a specialist in rigorous statistical mechanics [64–67]. His technical skills in cluster expansions will be very helpful in our tasks. Finally, there will be Siamak Taati in our team [68–70]. He is a former PhD student of Jarkko Kari, who constructed a minimal set of non-periodic tiles and a former postdoc of Aernout van Enter. Kari and Taati worked together on various problems in cellular automata. We would like to explore connections between non-periodic Gibbs states and stationary states of probabilistic cellular automata. Siamak Taati has already obtained some preliminary results in this direction. It is worth to add here that the connection between cellular automata and lattice-gas models are due to Christian Maes and others [12]. Christian Maes is a foreign investigator in Opus NCN grant on time delays in biological systems of which I am a principal investigator. Our topics there concern non-related to this project non-equilibrium statistical mechanics but we can expect some synergy here. Of course Christian Maes may also contribute to this project.

We will organize in Warsaw an opening meeting of our team. In the middle of the project a small working group meeting within a frame of Banach Center activities will be organized. There will be also a couple of pairwise meetings. The members of our team will communicate frequently through group skype conferences. We will have a dedicated web page to promote our results.

References

[1] G. E. Uhlenbeck, Statistical Mechanics; Foundations and Applications, ed. T. A. Bak, p. 581 (New York: Benjamin, 1967).

[2] G. E. Uhlenbeck, Fundamental Problems in Statistical Mechanics vol 2, ed. E. G. D. Cohen, p. 16 (New York: Wiley, 1968).

[3] B. Simon, Perspectives in Mathematics: Anniversary of Oberwolfach, p. 442 (Basel: Birkhauser, 1984).

[4] Anderson P W 1984 Basic Notions of Condensed Matter Physics, p. 11 (Menlo Park: Benjamin/Cummings 1984).

[5] C. Radin, Low temperature and the origin of crystalline symmetry, Int. J. Mod. Phys. B 1: 1157-1191 (1987).

[6] J. Miękisz, Quasicrystals - Microscopic Models of Nonperiodic Structures (Leuven Lecture Notes in Mathematical and Theoretical Physics, Vol. 5, Leuven University Press, 1993).

[7] A. C. D. van Enter, Aperiodicity in equilibrium systems: between order and disorder. Acta Physica Polonica A 126: 621-624 (2014).

[8] D. Schechtman, I. Blech, D. Gratias, and J. W. Cahn, Metallic phase with long-range orientational order and no translational symmetry, Phys. Rev. Lett. 53: 1951 (1984).

[9] P. Gacs, Reliable computation with cellular automata, Proceedings of the fifteenth annual ACM symposium on Theory of computing, 32-41 (1983).

[10] P. Gacs, Reliable cellular automata with self-organization, J. Stat. Phys. 103: 45267 (2001).

[11] L. Gray, A reader's guide to Gacs's positve rates paper, J. Stat. Phys. 103: 1-44 (2001).

[12] S. Goldstein, R. Kuik, J. L. Lebowitz, and C. Maes, From PCAs to equilibrium systems and back, Commun. Math. Phys. 125: 71-79 (1989).

[13] H. Wang, Proving theorems by pattern recognitionII, Bell System Technical Journal 40 (1): 141 (1961).

[14] R. Berger, The undecidability of the domino problem, Memoirs of the American Mathematical Society 66: 72 (1966).

[15] R. M. Robinson, Undecidability and nonperiodicity for tilings of the plane, Invent. Math. 12: 177-209 (1971).

[16] E. Jeandel and M. Rao, An aperiodic set of 11 Wang tiles, arXiv:1506.06492 (2015).

[17] R. Penrose, The role of aesthetics in pure and applied mathematical research, Bull. Inst. Math. Applications 10: 266 (1974).

[18] J. Miękisz, Classical lattice-gas models of quasicrystals, J. Stat. Phys. 97: 835-850 (1999).

[19] A C D van Enter, A Hof, and J. Miękisz, Overlap distributions for deterministic systems with many pure states, J. Phys. A Math. Gen. 25: L1133-Ll137 (1992).

[20] A. C. D. van Enter and J. Miękisz, How should one define a (weak) crystal? J. Stat. Phys. 66: 1147 (1992).

[21] M. Baake and U. Grimm, Can kinematic diffraction distinguish order from disorder? Phys. Rev. B 79: 020203 (2009).

[22] M. Baake and A. C. D. van Enter, Close-packed dimers on the line: diffraction versus dynamical spectrum, J. Stat. Phys. 143: 88-101 (2011).

[23] M. Baake, D. Lenz, and A. C. D. van Enter, Dynamical versus diffraction spectrum for structures with finite local complexity Ergodic Theory and Dynamical Systems 35: 2017-2043 (2015).

[24] M. Baake and U. Grimm, Aperiodic Order: Volume 1, A Mathematical Invitation (Encyclopedia of Mathematics and its Applications 149 Cambridge University Press, 2013).

[25] M. Keane, Generalized Morse sequences, Zeit. Wahr. 10: 3 35 (1968).

[26] J. Miękisz and C. Radin, The third law of thermodynamics, Mod. Phys. Lett. 1: 61-66 (1987).

[27] C. Gardner, J. Miękisz, C. Radin, and A. C. D. van Enter. Fractal symmetry in an Ising model, J. Phys. A, Math. Gen. 22: L1019 (1989).

[28] J. Miękisz, An ultimate frustration in classical lattice-gas models, J. Stat. Phys. 90: 285 (1998).

[29] S. Mozes, Tilings, substitution systems and dynamical systems generated by them, J. Anal. Math. 53: 139 (1989).

[30] L. Leuzzi and G. Parisi, Thermodynamics of a tiling model, J. Phys. A: Math. Gen. 33: (2001).

[31] H. Koch and C. Radin, Modelling quasicrystals at positive temperature, J. Stat. Phys. 138: 465-475 (2010).

[32] D. Aristoff and C. Radin, First order phase transition in a model of quasicrystals, J. Phys. A: Math. Theor. 44: 255001 (2011).

[33] Shin-ichi Sasa, Thermodynamic transition associated with irregularly ordered ground states in a lattice gas model, J. Phys. A: Math. Theor. 43 465002 (2010).

[34] C. Radin, Crystals and quasicrystals: a lattice gas model, Phys. Lett. A 114: 381 (1986).

[35] J. Miękisz, How low temperature causes long-range order, J. Phys. A: Math. Gen. 21: L529-L531 (1988).

[36] J. Miękisz and C. Radin, Why solids are not really crystalline? Phys. Rev. B 39: 1950-1952 (1989).

[37] J. Miękisz, Classical lattice gas model with a unique nondegenerate but unstable periodic ground state configuration, Commun. Math. Phys. 111: 533 (1987).

[38] R. L. Dobrushin and S. B Shloshman, The problem of translation invariance of Gibbs states at low temperatures, Soy. Sc. Rev. Sev. C, 5 (1985).

[39] J. Miękisz, A microscopic model with quasicrystalline properties, J. Stat. Phys. 58: 1137 (1990).

[40] J. Miękisz, Many phases in systems without periodic ground states, Commun. Math. Phys. 107: 577 (1986).

[41] T. W. Byington and J. E. S. Socolar, Hierarchical freezing in a lattice model, Phys. Rev. Lett. 108: 045701 (2012).

[42] S. Aubry, Weakly periodic structures and example, J. Phys. (Paris) Coll. C3-50: 97 (1989).

[43] W. H. Gottschalk and G. A. Hedlund , A characterization of the Morse minimal set, Proc. Amer. Math. Soc. 15: 70-74 (1964).

[44] J. Miękisz and C. Radin, The unstable chemical structure of the quasicrystalline alloys, Phys. Lett. A 119: 133 (1986).

[45] J. Aliste-Prieto, D. Coronel, and J.-M. Gambaudo, Rapid convergence to frequency for substitution tilings of the plane, Commun. Math. Phys. 306: 365-380 (2011).

[46] N. Ollinger, Two-by-two substitution systems and the undecidability of the domino problem, in Proc. Computability in Europe, LNCS 5028: 476-485 (2008).

[47] V. Poupet,Yet another aperiodic tile set, Journees Automates Cellulaires (Turku), 191-202 (2010).

[48] B. Durand, A. Romashchenko, and A. Schen, Fixed-point sets and their applications, J. Comp. and System Sciences 78: 731-764 (2012).

[49] A. C. D. van Enter and J. Miękisz, Breaking of periodicity at positive temperatures, Commun. Math. Phys. 134: 647 (1990).

[50] A. C. D. van Enter and B. Zegarliński, Non-periodic long-range order for one-dimensional pair interactions, J. Phys. A, Math. Gen. 30: 501 (1997).

[51] A. C. D. van Enter, J. Miękisz, and M. Zahradnik, Nonperiodic long-range order for fast-decaying interactions at positive temperatures, J. Stat. Phys. 90: 1441 (1998).

[52] M. Mendès-France, Review of " An ultrametric state space with dense discrete overlap distribution: paperfolding sequences", by A.C.D. van Enter and E. de Groote, Math. Rev., MR2764124 (2012).

[53] J. Jędrzejewski and J. Miękisz, Ground states of lattice gases with "almost" convex repulsive interactions, J. Stat. Phys. 98: 589-620 (2000).

[54] P. Bak and R. Bruinsma, One-dimensional Ising model and the complete devil's staircase, Phys. Rev. Lett. 49: 249 (1982).

[55] S. Aubry, Exact models with a complete devil's staircase, J. Phys. C 16: 2497 (1983).

[56] R. Lifshitz, The square Fibonacci tiling, J. Alloys and Compounds 342: 186-190 (2002).

[57] P. R. Halmos, In general a measure-preserving transformation is mixing, Ann. Math. 45: 786-792 (1944).

[58] V. Rohlin, A "general" measure-preserving transformation is not mixing, Dokl. Akad. Nauk, SSSR (N.S.) 60: 349–351 (1948).

[59] B. Simon, Operators with singular continuous spectrum: I. General operators, Ann. Math. 141: 131–145 (1995).

[60] A. L. Toom, Nonergodic multidimensional systems of automata, Problems Inform. Transmission 10: 239-246 (1974).

[61] P. Gacs and J. Reif, A simple three-dimensional real-time reliable cellular array, J. Comp. and System Sciences 36: 125-147 (1988).

[62] S. A. Pirogov, and Ya. G. Sinai, Phase diagrams of classical lattice systems, Teor. Mat. Fiz. 25: 358-369 (1975).

[63] S. A. Pirogov, and Ya. G. Sinai, Phase diagrams of classical lattice systems, Teor. Mat. Fiz. 26: 61-76 (1976).

[64] M. Biskup, On the scaling of the chemical distance in long range percolation models, Ann. Probab. 32: 2938-2977 (2004).

[65] M. Biskup and R. H. Schonmann, Metastable behavior for bootstrap percolation on regular trees, J. Stat. Phys. 136: (2009), no. 4, 667-676 (2009).

[66] M. Biskup and R. Kotecký, Phase coexistence of gradient Gibbs states, Probab. Theory Rel. Fields 139: 1-39 (2007).

[67] M. Biskup and O. Louidor, Extreme local extrema of two-dimensional discrete Gaussian free field, Commun. Math. Phys. 345: 271–304 (2016).

[68] A. van Enter, G. Iacobelli, and S. Taati, Potts model with invisible colours: Random-cluster representation and Pirogov-Sinai analysis, Rev. Math. Phys. 24: 1250004 (2012).

[69] S. Taati, Restricted density classification in one dimension, Proceedings of AUTOMATA-2015, LNCS 9099, 238–250, Springer (2015).

[70] J. Kari and S. Taati, Statistical mechanics of surjective cellular automata, J. Stat. Phys. 160: 1198–1243 (2015).