XLI WORKSHOP ON GEOMETRIC METHODS IN PHYSICS

1—6 JULY 2024, BIAŁYSTOK, POLAND

Ergodic theory and topology of nonperiodic tilings and Gibbs states of interacting particles

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Main Open Problem

Does there exist a lattice-gas model
with translation-invariant finite-range interactions,
without periodic ground-state configurations
and with non-periodic Gibbs states at low temperatures
which are small perturbations
of non-periodic ground-state configurations ?

A short history of quasicrystals

David Hilbert 1862 - 1943

23 problems, 1900

Problem 18 Part II

Does there exist a polyhedron which can cover the space
but only in a nonperiodic way ?

Hao Wang 1921 - 1995

Hilbert problem for domino players

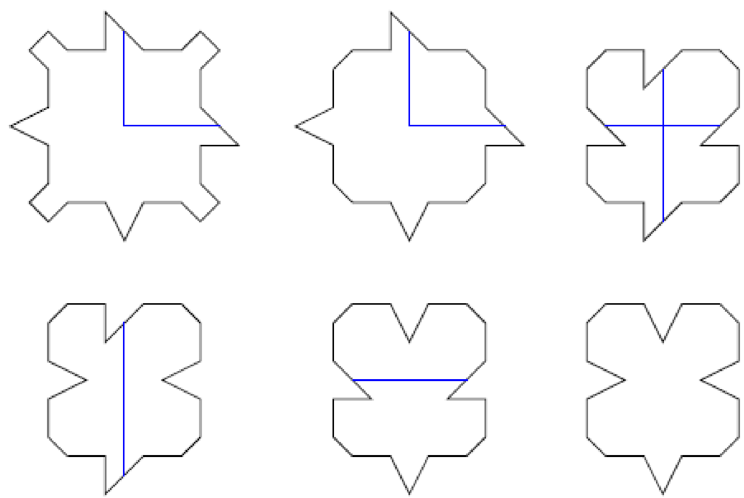
Wang tiles ---- squares with colored sides ---- square dominoes

Wang Hypothesis 1961

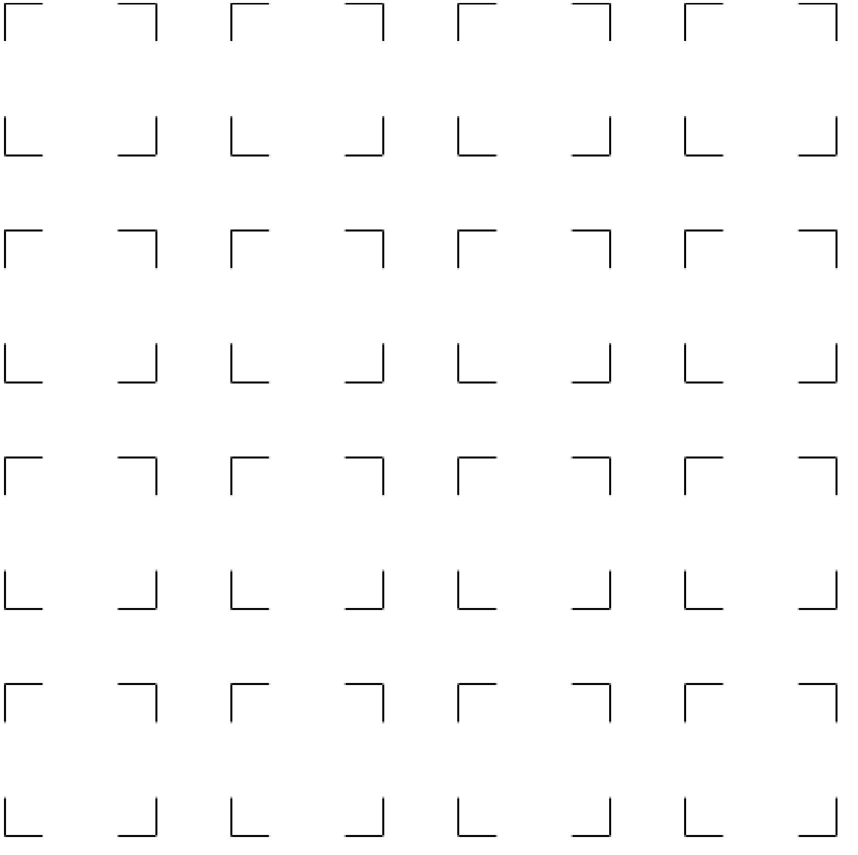
Each finite set of dominoes which covers the plane,
may also cover it in a periodic way.

Raphael Robinson 1911 - 1995

6 (56) tiles which cover planes but only in a non-periodic way, 1971



Structure of an infinite tiling



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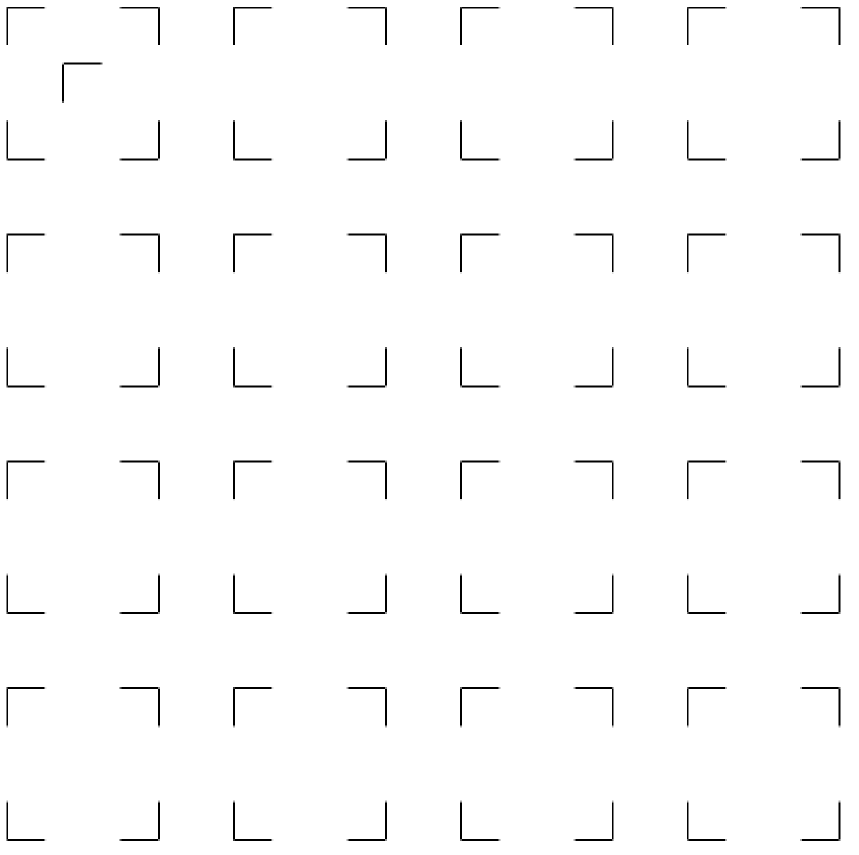

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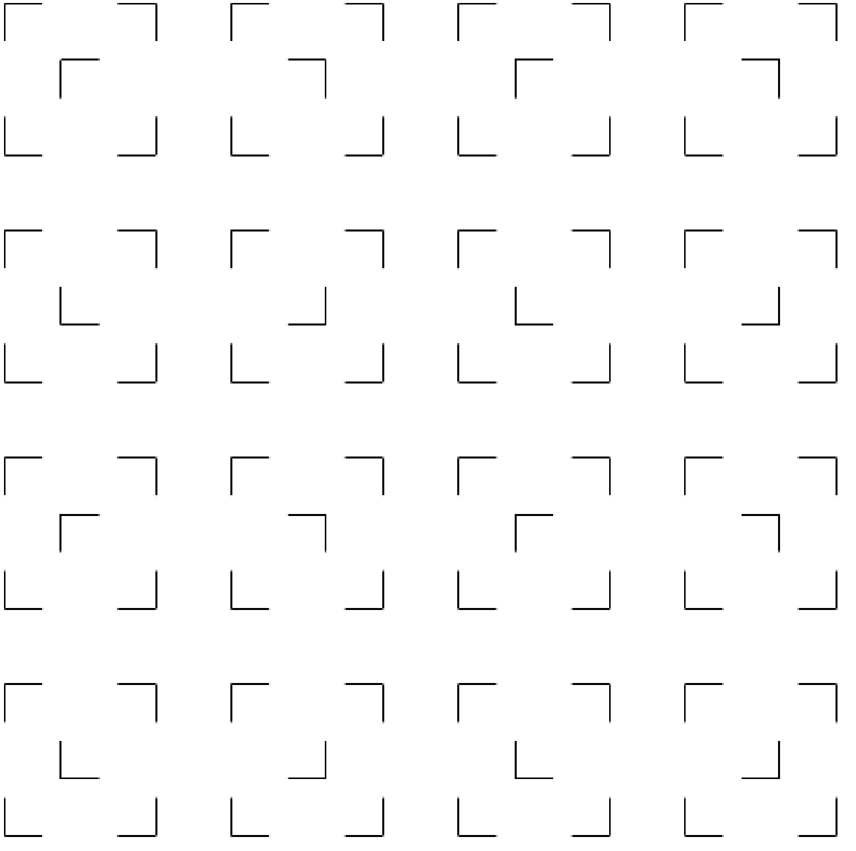

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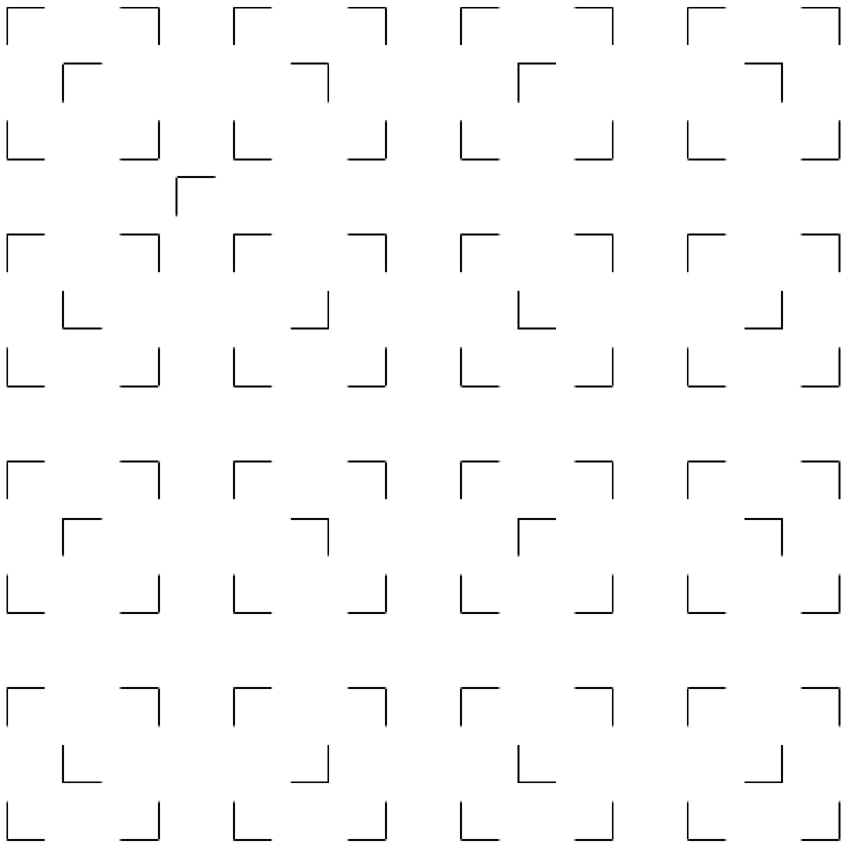

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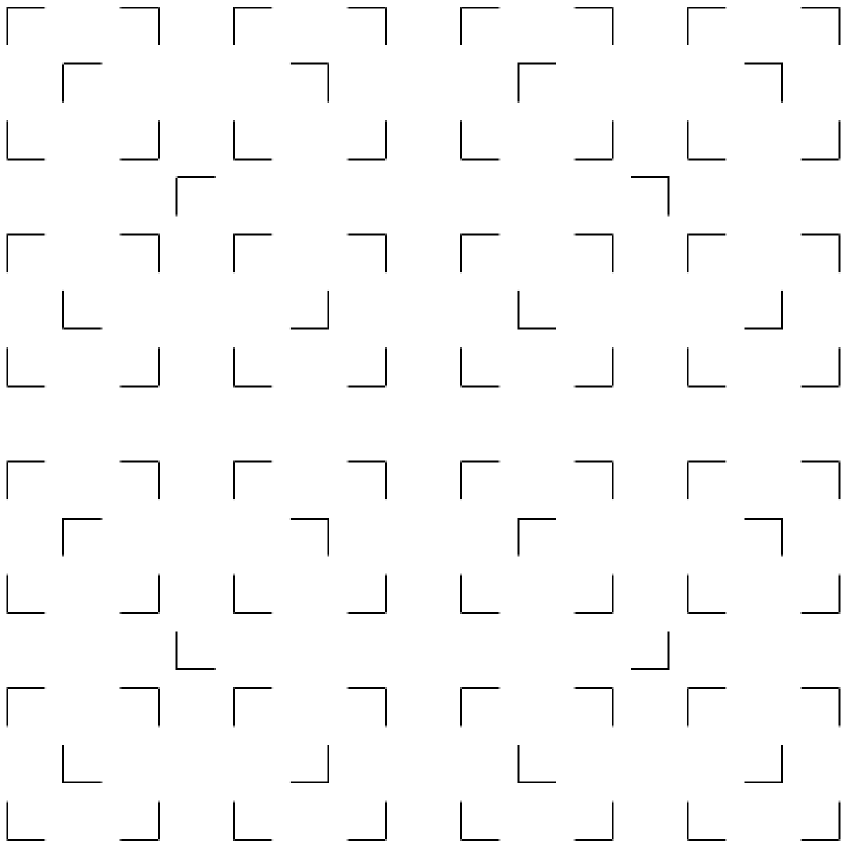

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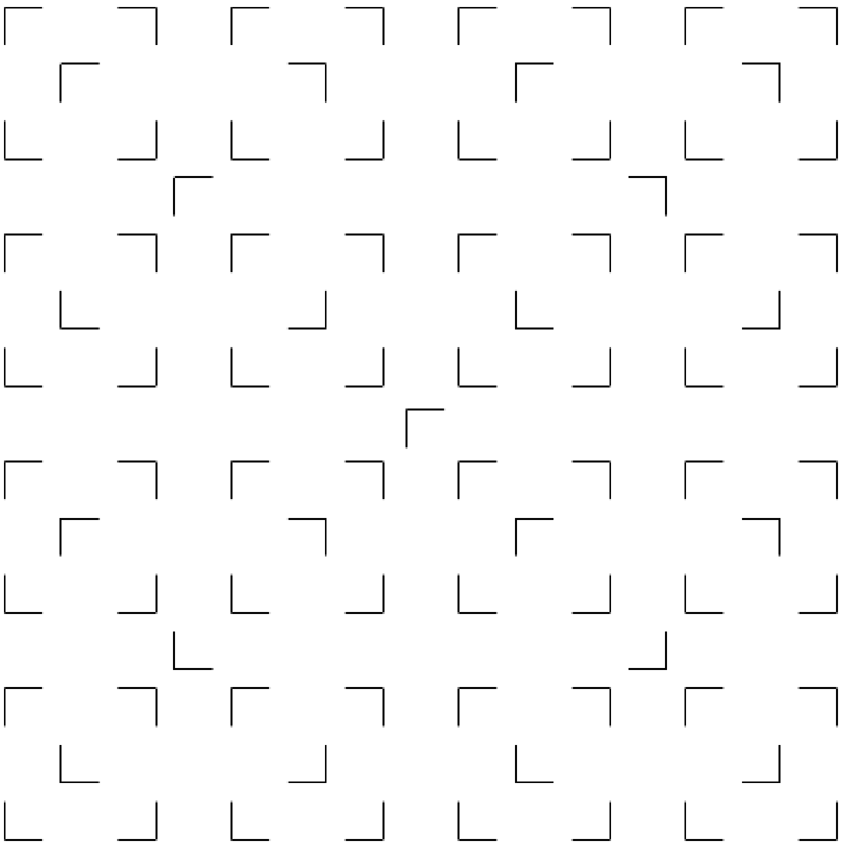


Configurations with period 2^{n+1} on sublattices $2^n Z^2$ $n \geq 1$

Global order from local rules

Properties of Robinson's tilings

1. There are uncountably many tilings.

2. Every local pattern can be extended to an infinite tiling in uncountably many ways.

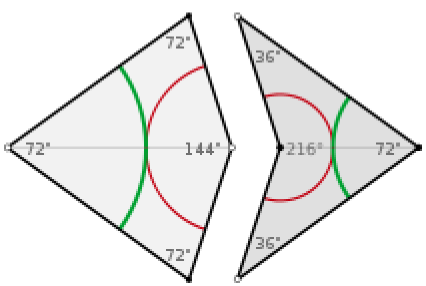
3. Every local pattern appears with the same frequency in all Robinson's tilings.

4. Robinson' s tilings are locally indistinguishable.

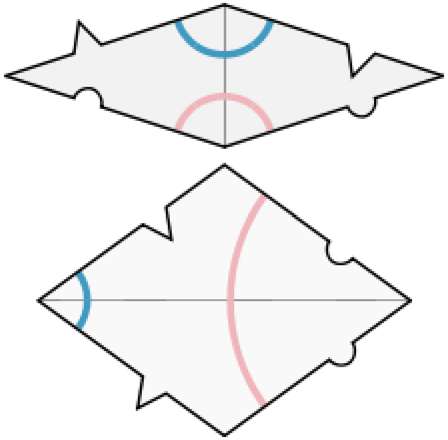
Roger Penrose 1931 -

Two tiles which cover the plane but only in non-periodic way, 1974

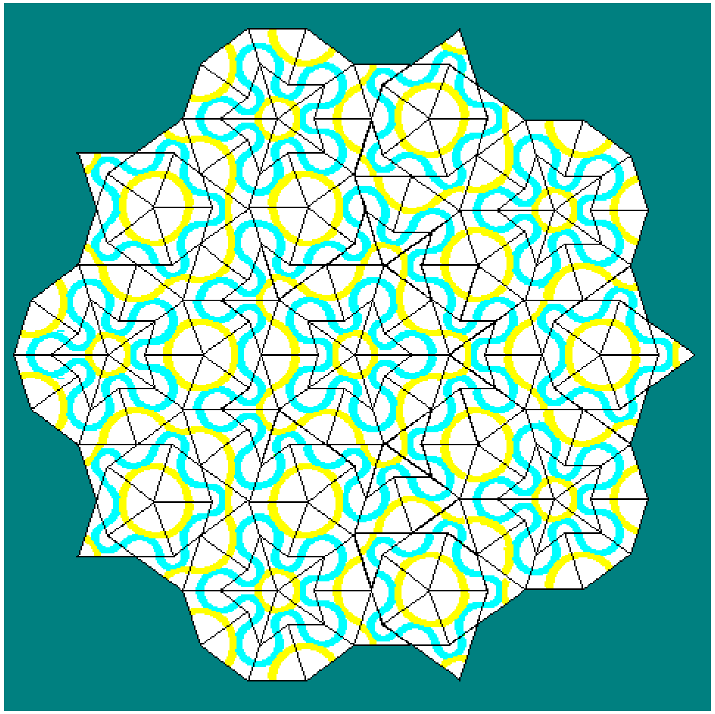
dart and kite

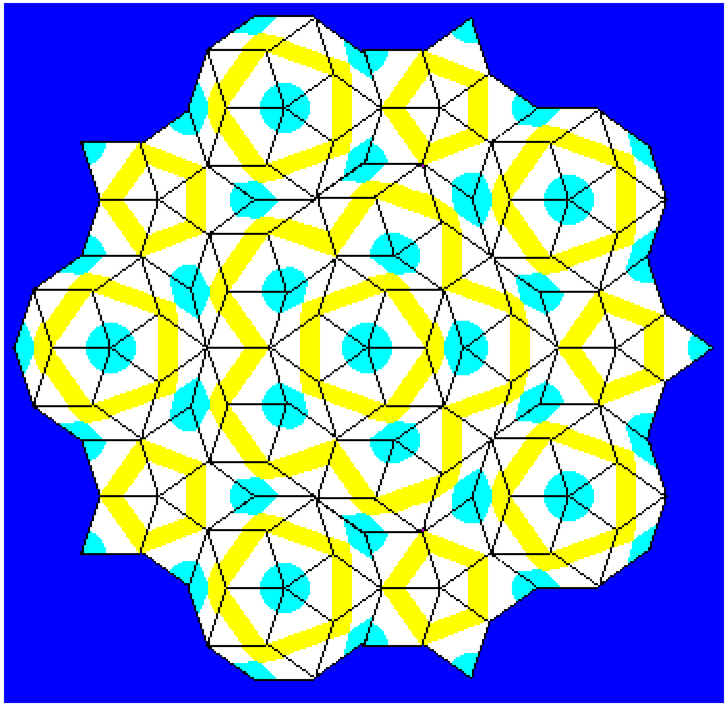


rhombs



Penrose tilings



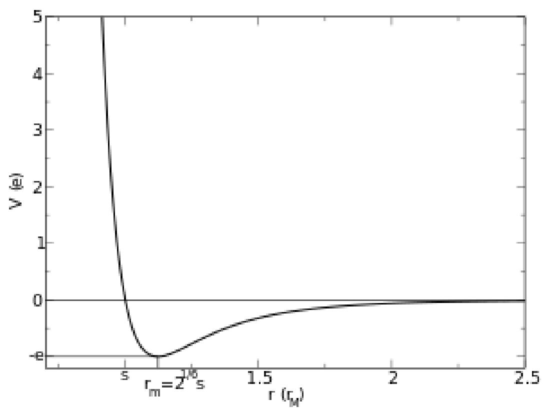


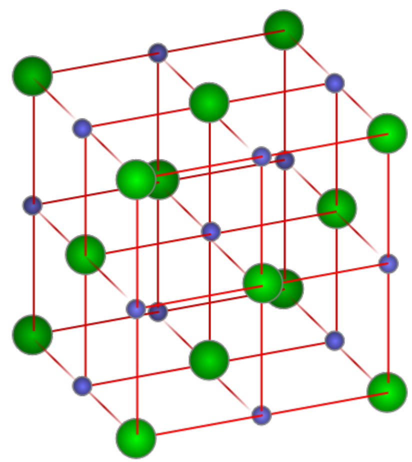
Steven Dutch, Natural and Applied Sciences, University of Wisconsin - Green Bay

The Crystal Problem

Equilibrium state of many interacting particles
minimizes free energy $F = E - TS$
(or energy E in temperature $T = 0$)

To prove that minimization of the energy of realistic particle interactions, for example Lennard-Jones, leads to periodic crystal lattices.



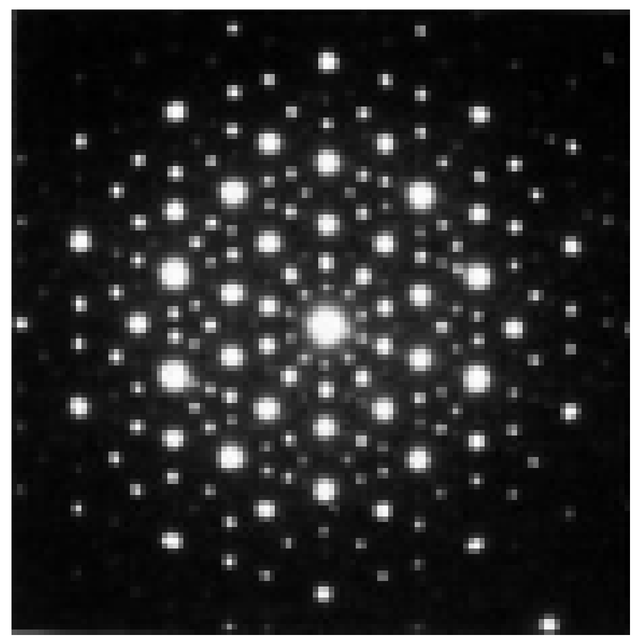


Dan Shechtman 1941 -

Technion Israel Institute of Technology
Iowa State University

8 April 1982 in National Bureau of Standards in Washington

Dan Shechtman was observing rapidly solidified aluminum transition metal alloys



Nobel Prize in Chemistry, 2011

Philip W. Anderson

Basic notions of condensed matter physics, 1984

Benjamin/Cummings Pub. Co.

„Proved” that every interaction has at least one periodic ground-state configuration

Classical lattice-gas models based on tilings

tiles $\rightarrow$ particles

matching rules $\rightarrow$ interactions

If two tiles do not match, then the energy of interaction between corresponding particles is positive, say 1, otherwise the energy is zero

ground-state configurations – configurations which minimize the energy

forbidden patterns have positive energy

tilings $\rightarrow$ ground-state configurations

ground-state configurations have zero energy

Overview

Physical space: $\mathbf{Z}^d, d = 1, 2$

Space of configurations: $\Omega = \{1, ..., n\}^{\mathbf{Z}^d}$

Non-periodic configurations in $\Omega \to$ ground-state configurations of some Hamiltonians

d=2, nonperiodic tilings (Robinson's tilings),
in general systems of finite type

d=1, substitution dynamical systems (Thue-Morse sequences),
Sturmian systems (Fibonacci sequences),
in general systems of minimal infinite type

Main theme: stability of nonperiodic ground states

Zero-temperature stability

μ_G is the ground-state measure of H.

Is μ_G the ground-state measure of $H + \epsilon H'$ for some small ϵ?

Negative example

Lattice-gas model based on Robinson's tilings has the unstable non-periodic ground state.

(Międkisz and Radin, Phys. Lett. 1985)

Low-temperature stability

Let H be a finite-range Hamiltonian with a unique non-periodic ground-state measure (based for non-periodic tilings for example)

Let $X \in \Omega$ be one of its ground-state configurations, Λ_L be a square of size L centered at the origin.

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

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

is a finite-volume Gibbs measure, $\beta = 1/T$, T is the temperature of the system.

One can show that

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

We would like to prove that

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

$$\epsilon(\beta) \to 0 \;\; as \;\; \beta \to \infty$$

ρ^X_T would be then a non-periodic Gibbs state, a perturbation of non=periodic ground-state measure.

Open Problem

Does there exist a lattice-gas model with translation-invariant finite-range interactions without periodic ground-state configurations and non-periodic equilibrium state at positive temperature ?

so far

Theorem (JM, 1990)

There is a decreasing sequence of temperatures, T_n, such that if $T < T_n$, then there exists a Gibbs state with a period at least 2×6^n in both directions.

nonperiodic Gibbs states

van Enter, Miękisz, CMP 1990
nonperiodic Gibbs states for summable interactions

van Enter, Miękisz, Zahradnik, JSP 1998
nonperiodic Gibbs states for exponentially decaying interactions

General features of all models considered here

We will discuss the following systems:

$$(\Omega, H, G, T, \mu_G),$$

$G \subset \Omega$ is the set of non-periodic ground-state configurations of the Hamiltonian H,

there are no periodic ground-state configurations.

$(T_a X)_i = X_{i-a}; a, i \in \mathbf{Z}^d \quad X \in G$

$G = closure\{T_a X, a \in \mathbf{Z}^d\}$ in the product topology

G is uniquely defined by a set of **forbidden patterns**, a finite set in $d = 2$ and an infinite set in $d = 1$.

There exists the unique translation-invariant measure μ_G on G, **called a ground-state measure**

$\mu_G = \lim_{L \to \infty} \frac{1}{L^2} \sum_{a \in \Lambda_L^0} \delta_{T_a X},$

where $\delta_{T_a X}$ is a probability measure which assigns 1 to $T_a X$ and Λ_L^0 is the hypercube centered at the origin with the side lenght L.

30-year anniversary

Alain Connes

Noncommutative Geometry

Academic Press 1994

Preliminary observation – Robinson's tiling

Let G be set of Robinson' s tilings, a compact subset of Ω

We say that two tilings are equivalent if they are related by translation, we denote the equivalence relation by R

What is the topology on G/R, the set of equivalence classes?

Now we apply Connes ideas to Fibonacci sequences.

Fibonacci sequences

substitutions

0 → 01
1 → 0

0	1
01	2
010	3
01001	5
01001010	8
0100101001001	13

$(F, T, \mu F)$ *is a uniquely ergodic system*

density of 0's = $\dfrac{2}{1+\sqrt{5}} = \gamma$

Another construction of Fibonacci sequences

Let $0 \leq \phi \leq 2\pi$ and let T_γ be a rotation by $2\pi\gamma$ on a unit circle.

If $T_\gamma^n(\phi) \in [0, 2\pi\gamma)$ *mod* 2π then let $a(n) = 0$, otherwise $a(n) = 1$.

Self-similarity of Fibonacci sequences

$X \in F$

$01 \to 0$
$0 \to 1$

$X \to Y_X \in F$

We repeat groupings and obtain a coding of X by a sequence $z_n, n \geq 1$ such that $z_n z_{n+1} = 0$.

Two Fibonacci sequences X, X' are equivalent (related by a translation) iff there is k such that $z_j = z'_j$ for every $j \geq k$.

Again, the space of tilings, $S = F/R$, has a trivial topology.

Let A be a matrix $a_{zz'}$ indexed by pairs $(z, z') \in R$.

For $x \in S$, there is an equivalence class of R - a countable subset of F.

We associate to x the Hilbert space l^2_x.

Every element a of A defines an operator on l^2_x,

$$(a(x)f)_z = \sum_{z'} a_{zz'} f_{z'}, f \in l^2_x.$$

A is a C^* algebra with the operator norm $||a(x)||$.

Strict Boundary Property of nonperiodic tilings (nonperiodic configurations in general) [1,2]

$X \in \Omega$ satisfies the **Strict Boundary Property** for a local pattern ar if there is a constant C_{ar} such that

$$|n_{ar}^{L}(X) - \omega_{ar}L^{2}| < C_{ar}L.$$

Such property is also called a rapid convergence to equilibrium of frequency of patterns [3,4].

In fact we need a following stronger version for local tilings.

Let $W \subset \Omega$ be a set of nonperiodic tilings for a given tiling set such that there is the unique translation-invariant probability measure supported by tilings.

W satisfies the **Strict Boundary Property** for a local pattern ar if for any local tiling Y of Λ_{L}^{0}, not necessarily extendable to the whole $\mathbf{Z}^{2}$

$$|n_{ar}^{L}(Y) - \omega_{ar}L^{2}| < C_{ar}L.$$

Theorem (J. Miękisz, J. Stat. Phys.1997 [1])

A unique ground-state measure of a finite-range Hamiltonian is stable against small perturbations of interactions of range smaller than r if and only if Strict Boundary Property is satisfied for patterns of diameter smaller than r

Theorem (J. Miękisz, C. Radin, Phys. Lett. 1986) [7])

Robinson's ground state is not stable against
an arbitrarily small chemical potential favoring
one type of particles corresponding to an arrow tile.

One-dimensional lattice-gas models

It is known that one-dimensional lattice-gas models with finite-range interactions have at least one periodic ground-state configuration.

(Miękisz and Radin, Mod. Phys. Lett. 1987)

Therefore to force nonperiodicity we have to consider models with infinite-range potentials.

Sturmian ground-state measure

We build Sturmian sequences by rotations on the unit circle.

We will identify the circle C with $R/\mathbb{Z}$ and consider an irrational rotation by φ which is given by translation on $R/\mathbb{Z}$ by φ mod 1.

Given an irrational $\varphi \in C$ we say that $X \in \{0,1\}^{\mathbb{Z}}$ is generated by φ if it is of the following form:

$$X(n) = \begin{cases} 0 & \text{when } x + n\varphi \in P \\ 1 & \text{otherwise} \end{cases}$$

where $x \in C$ and $P = [0, \varphi)$.

Sturmian sequences can be characterized by absence of certain finite patterns.

Let $\varphi \in (\frac{1}{2}, 1)$ be irrational. Then there exists a natural number m and a set $F \subseteq \mathbb{N}$ of forbidden distances such that Sturmian sequences generated by φ are uniquely determined by the absence of the following patterns: m consecutive 0's and two 1's separated by a distance from F.

Two-body interactions were constructed for which ground states are supported by Sturmian sequences.

(van Enter, Koivusalo, Miękisz, J. Stat. Phys. 2021)

Example Fibonacci ground state

$\varphi = \frac{2}{1+\sqrt{5}}$

Forbidden distances between 1's = 1,4,9,12,17,22,25,30,...
we also forbid 000.

Theorem 2 (Głodkowski, Miękisz, arXiv preprint, 2024)

Sturmian ground states generated by rotation by badly approximable irrationals with $f(r) \sim \frac{1}{r^{\alpha}}$ for $\alpha > 3$ are unstable with respect to an arbitrarily small chemical potential favoring the presence of particles.

We say that a number φ is **badly approximable** if there exists $c > 0$ such that

$$\left|\varphi - \frac{p}{q}\right| > \frac{c}{q^2}$$

for all rationals $\frac{p}{q}$.

Open problem

Are Sturmian ground states stable for $\alpha < 3$?

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[7] D. Głodkowski and J. Miękisz, On non-stability of one-dimensional non-periodic ground states, https://arxiv.org/abs/2401.11594

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Mathematical models of quasicrystals

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