Baby Steps Beyond the Horizon:
Mathematics for Students, Będlewo

7 September 2021

Mathematical physics of quasicrystals

Jacek Miękisz
Institute of Applied Mathematics and Mechanics
University of Warsaw

From Hilbert to Shechtman

a short strongly biased history of non-periodicity

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

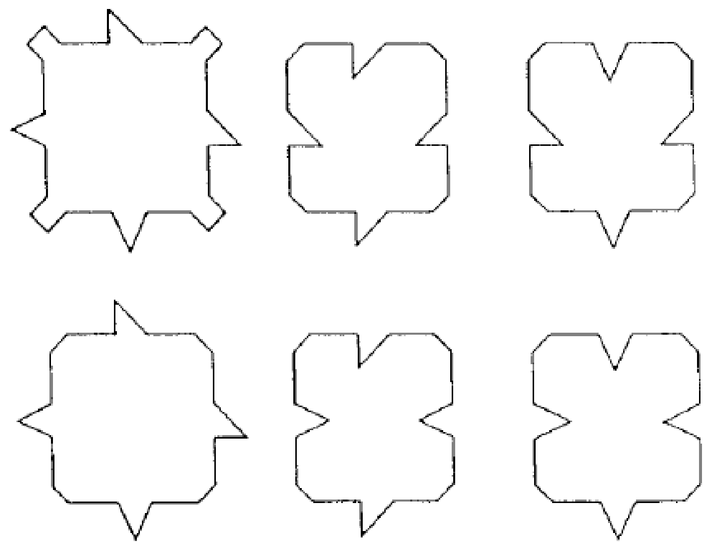
Wang tiles ---- squares with colored sides ---- square dominoes

Wang Hypothesis 1961

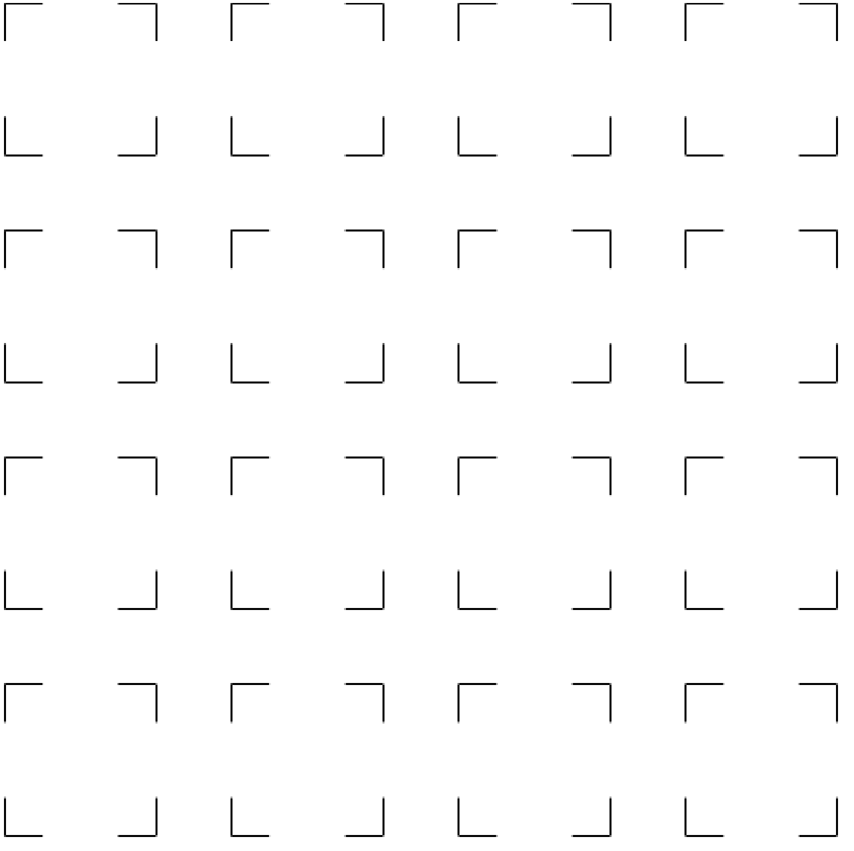
Each finite set of dominoes which covers the plane,
may also cover it in a periodic way.

Raphael Robinson 1911 - 1995

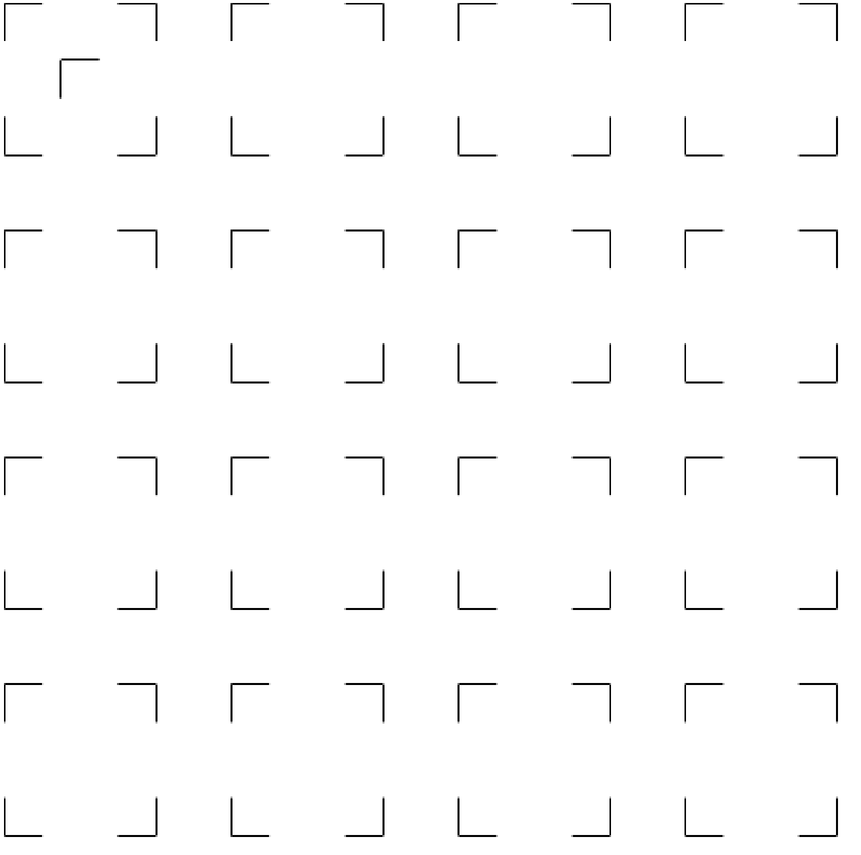
6 (56) tiles which cover planes but only in a non-periodic way, 1971



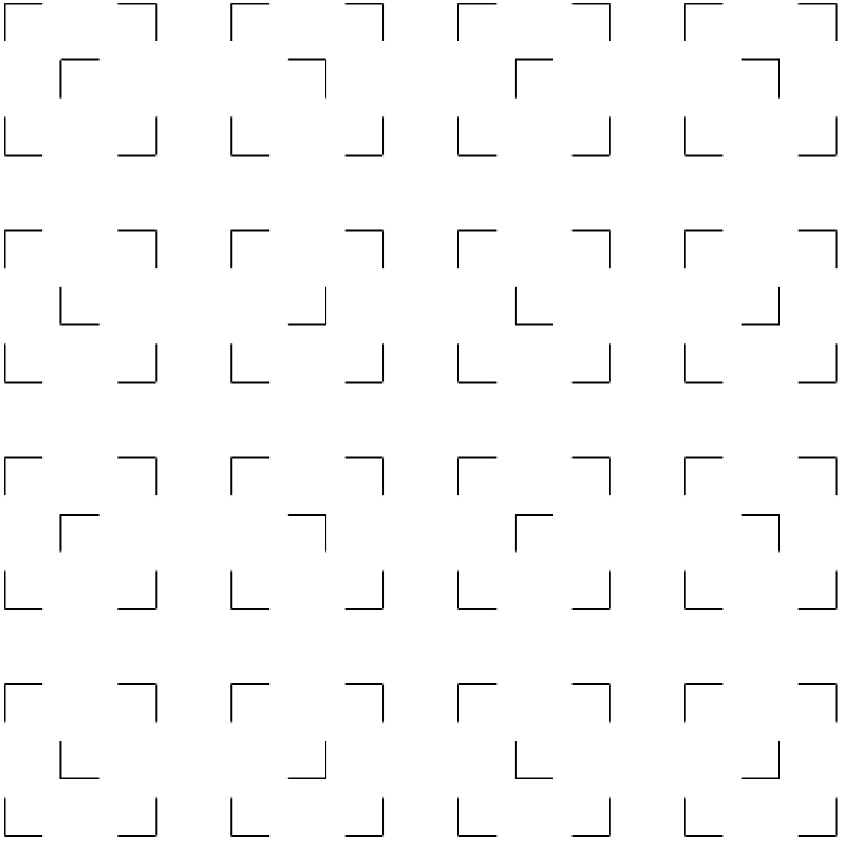
Structure of an infinite tiling



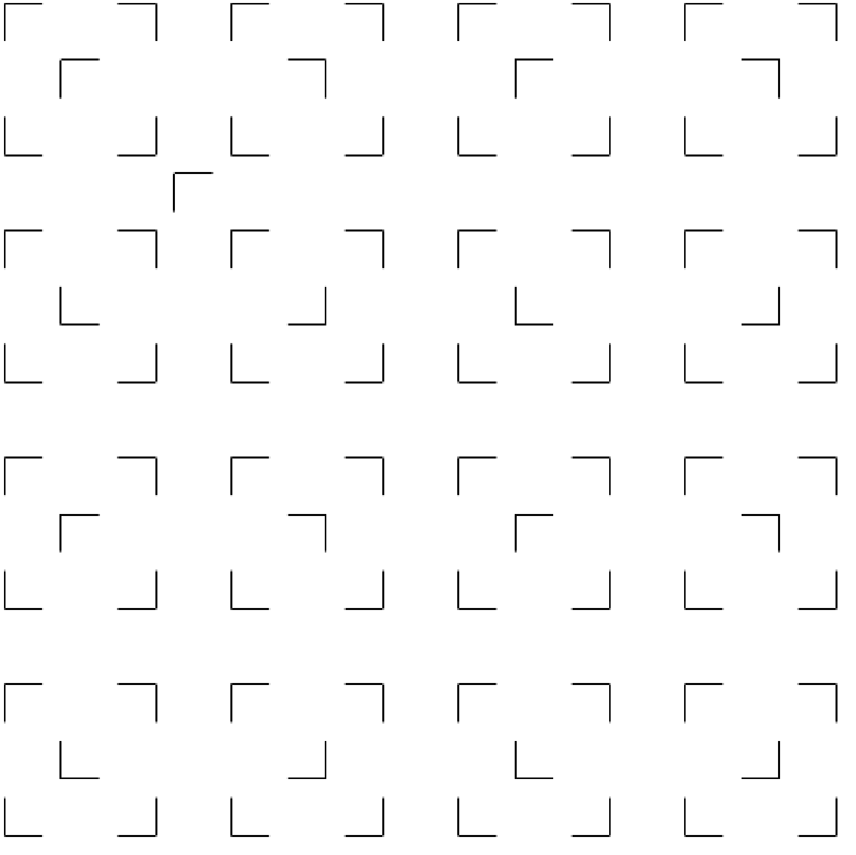
Structure of an infinite tiling



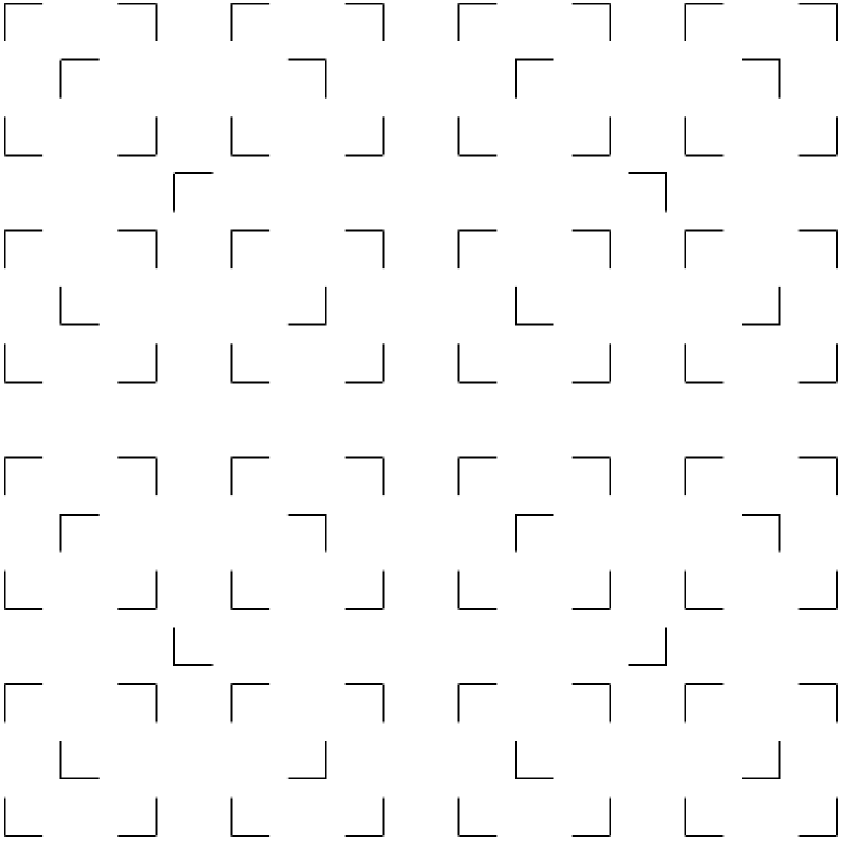
Structure of an infinite tiling



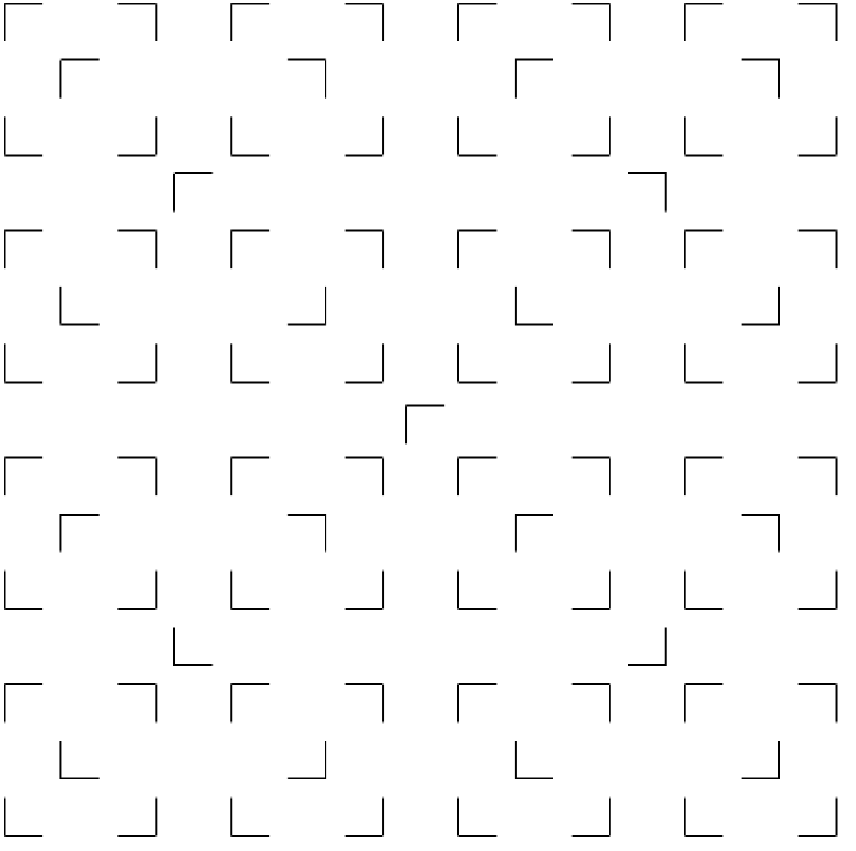
Structure of an infinite tiling



Structure of an infinite tiling

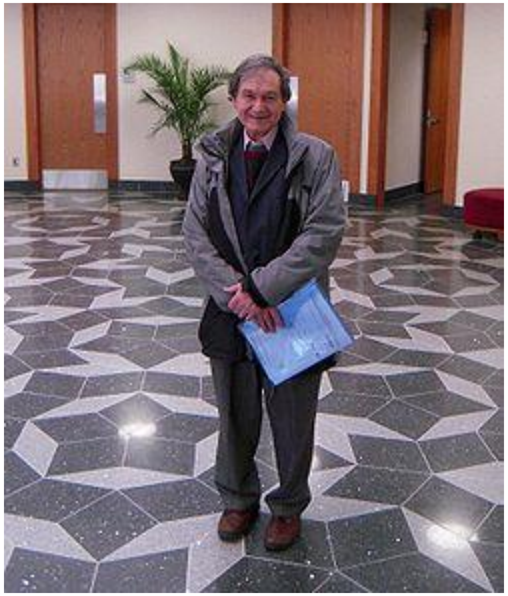


Structure of an infinite tiling



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

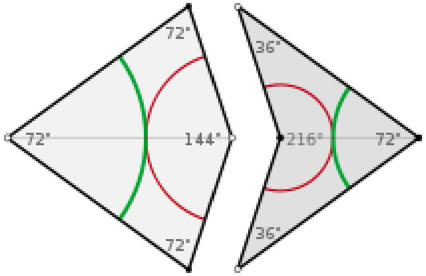
Global order from local rules



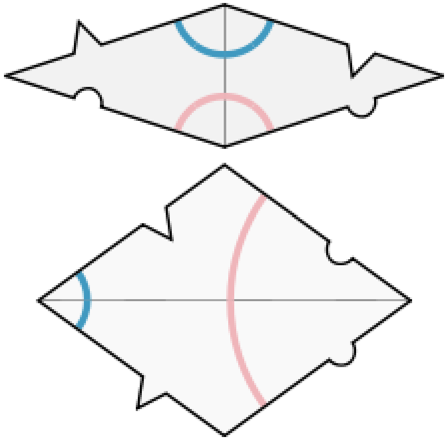
Roger Penrose 1931 -

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

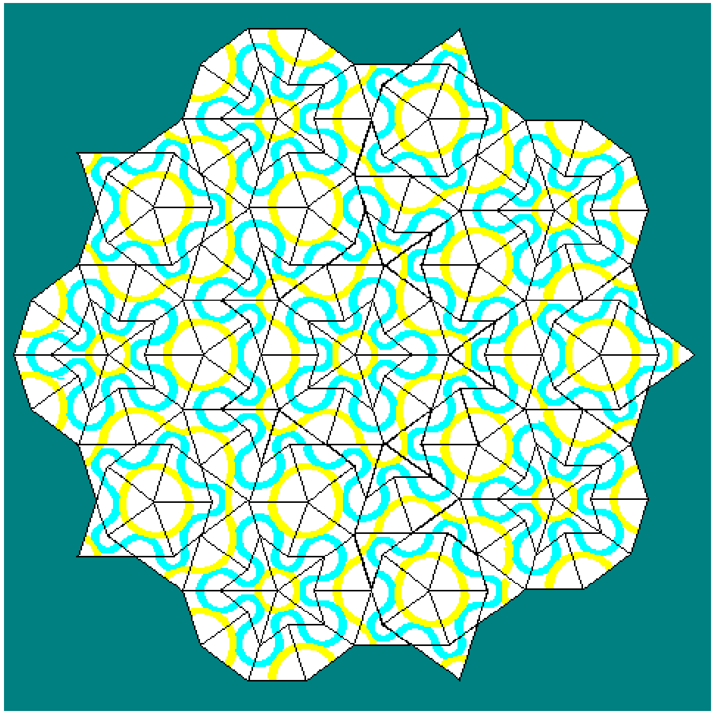
dart and kite

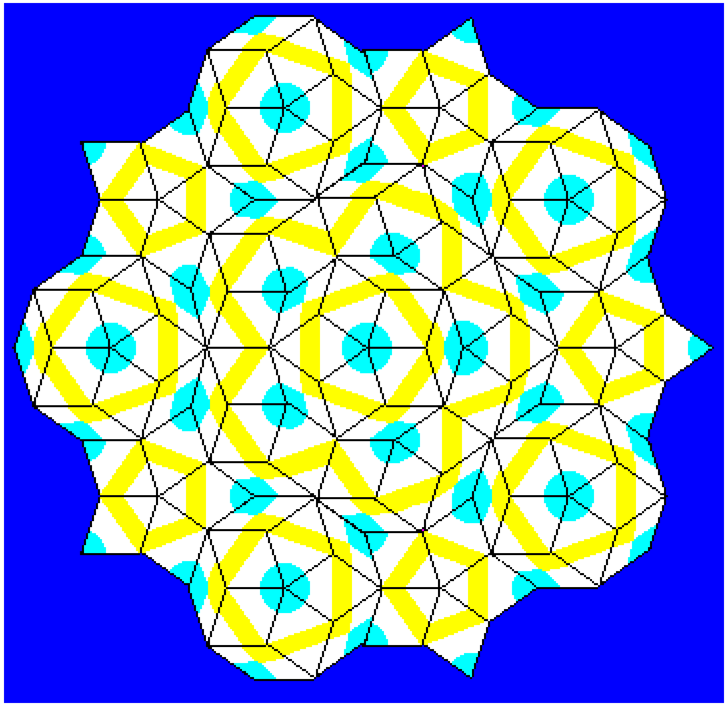


rhombs



Penrose tilings





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

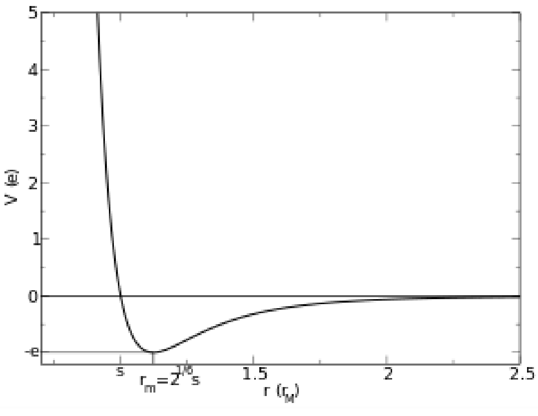
The Crystal Problem

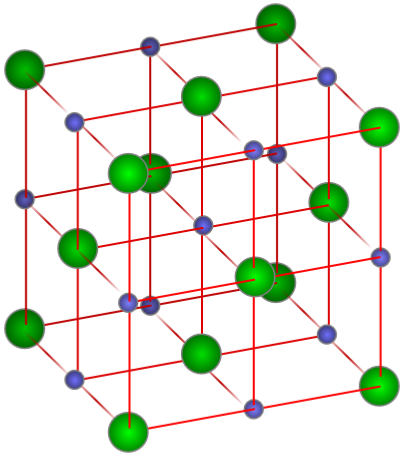
The fundamental law of physics

The Nature is lazy

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.





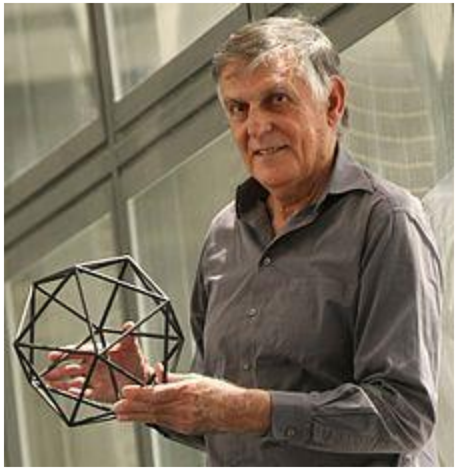
Philip W. Anderson

Basic notions of condensed matter physics, 1984

Benjamin/Cummings Pub. Co.

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

https://www.mimuw.edu.pl/~miekisz/

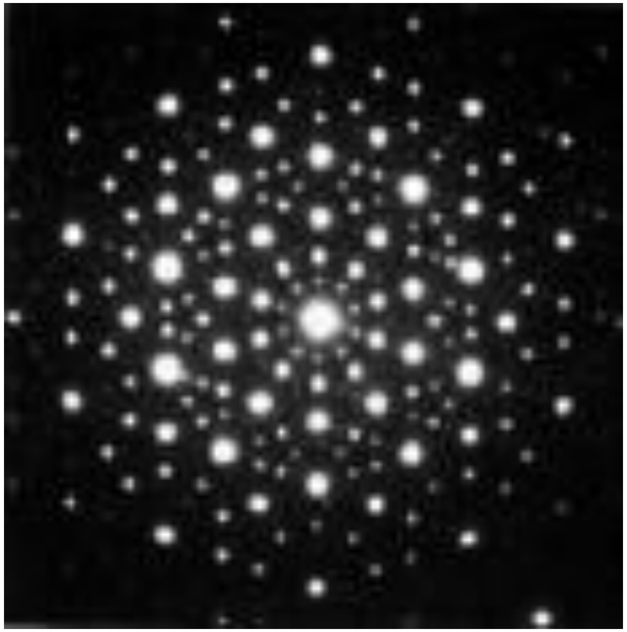


Dan Shechtman 1941 -

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

Lattice-gas models

and

dynamical systems of finite type

Ground-state configurations

There are n types of particles.

Every site of Z^d, $d \geq 1$, is occupied by one particle.

$\Omega = \{1, ..., n\}^{Z^d}$ is the set of all particle configurations.

For a finite subset $\Lambda \subset Z^d$, $\Omega_\Lambda = \{1, ..., n\}^\Lambda$.

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

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

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

Φ is **translation-invariant potential** if $\Phi_{\Lambda+a}(\tau_a X) = \Phi_\Lambda(X)$

for every $a \in Z^d$, where τ_a is translation by vector a that is $(\tau_a X)_i = X_{i-a}$.

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

$$H_\Lambda^\Phi : \Omega_\Lambda \to R$$

Example Ising model

$$\Omega = \{+1, -1\}^{Z^d}, X \in \Omega, \sigma_i(X) = X_i, i \in Z^d$$

$$H_\Lambda = - \sum_{<i,j>, i,j \in \Lambda} \sigma_i \sigma_j - h \sum_{i \in \Lambda} \sigma_i, \quad h > 0$$

Topology on Ω

The smallest topology such that all projections $\sigma_i : \Omega \to \Omega_i = \{+1,-1\}$ are continuous, with {+1,-1} equipped with the discrete topology.

Exercise 1

Characterize the convergence $X(n) \to X$ on Ω

We would like to minimize the energy of configurations

$$e(X) = liminf_{\Lambda \to Z^d} \frac{H_\Lambda^\Phi}{|\Lambda|} \quad \text{energy density of } X \in \Omega$$

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

For $Y \sim X$, **relative Hamiltonian** is defined as

$$H^\Phi(Y|X) = \sum_{\Lambda \subset Z^d} (\Phi_\Lambda(Y) - \Phi_\Lambda(X)).$$

$X \in \Omega$ is a **ground-state configuration** for potential Φ

if for every local excitation, $Y \sim X$, $H^\Phi(Y|X) \geq 0$.

Exercise 2

Prove that ground-state configurations minimize energy density

Exercise 3

Prove that every translation-invariant finite-range interaction has at least on ground-state configuration.

Exercise 4

Find all ground-state configurations in the ferromagnetic Ising model with $h=0$, in dimensions $d=1$ and $d=2$.

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

Gibbs measures

Finite-volume Gibbs measures

$\Lambda \subset Z^d$ is finite, $H_\Lambda : \Omega_\Lambda \to R$ is a finite-volume Hamiltonian,

$\rho_\Lambda^\Phi = \frac{e^{-\beta H_\Lambda}}{Z_\Lambda}$

is a finite-volume Gibbs state (Gibbs measure, grand-canonical ensemble),

$Z_\Lambda = \Sigma_{X \in \Omega_\Lambda} e^{-\beta H_\Lambda(X)}$

is a statistical sum, $\beta = 1/T$ is the inverse temperature.

Let M_Λ be the set of all probability measures on Ω_Λ and let $\rho \in M_\Lambda$.

$S(\rho) = E_\rho(\ln \rho)$ is the entropy functional,

$F_\Lambda(\rho) = E_\rho(H_\Lambda) + TE_\rho(\ln \rho)$ is the free energy functional (pressure).

Proposition

ρ_Λ^Φ minimizes F_Λ,

$F_\Lambda(\rho_\Lambda^\Phi) = -T \ln Z_\Lambda$

Infinite-volume Gibbs measures

Thermodynamic limit

$$f^{\Phi} = \lim_{\Lambda \to Z^d} \frac{F_{\Lambda}(\rho_{\Lambda}^{\Phi})}{|\Lambda|}$$

Let $X \in \Omega = \{1, ..., n\}^{Z^d}$ and Λ_L be the hypercube of size L centered at the origin.

$$\Omega_{\Lambda_L}^{X} = \{Y \in \Omega, Y(\Lambda_L^c) = X(\Lambda_L^c)\}$$

$$\rho_{\Lambda}^{X}(Y) = \frac{e^{-\beta H(Y,X)}}{Z_{\Lambda}^{X}}$$

Infinite-volume Gibbs measures are weak limits as $L \to \infty$ of ρ_{Λ}^{X} for all $X's$.

Back to quasicrystals

Let H be a Hamiltonian associated with a non-periodic tiling system.

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

We would like to prove that

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

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

ρ^X would be then a non-periodic Gibbs measure - a small perturbation of the ground-state measure.

Some results

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.

The existence of non-periodic Gibbs states was proven for

a) summable interactions (A. van Enter, JM, CMP, 1990)

b) exponentially decaying interactions (A. van Enter, JM, M. Zahradnik, JSP, 1998)

Systems of finite type

$$\Omega = \{1, ..., 56\}^{Z^2}$$

Let X be a Robinson's tiling, $X \in \Omega$

$$R = closure(\{T_a X, a \in Z^2\})$$

$$\mu_R = lim_{\Lambda \to Z^2} \frac{1}{|\Lambda|} \Sigma_{a \in \Lambda} \delta_{T_a} X$$

R is defined by a finite number of forbidden patterns – two neighboring tiles that do not match

(R, T, μ_R) is a dynamical system of finite type

μ_R is a uniquely ergodic measure.

systems of finite type ---> lattice-gas models with finite-range interactions

ergodic measure ----- ground-state measure

However

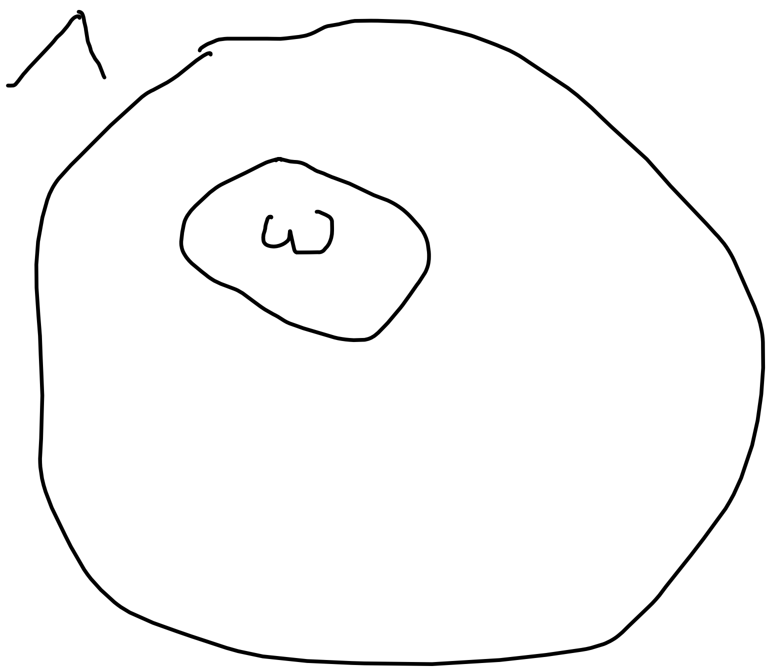
Lattice-gas models with finite-range interactions
are not necessarily dynamical systems of finite type

JM, Journal of Statistical Physics, 1999

Let X_R be any Robinson's tiling.

$\Lambda \in Z^2$ is a finte set and P its boundary, n_{ar} the number of appearence of some finite pattern ar in X_R on Λ

$$\frac{n_{ar}}{|\Lambda|} \to \omega_{ar} \; when \; \Lambda \to Z^2$$



Does there exist a non-periodic system of finite type such that the following Strict Boundary Condtion is satisfied

$$|n_{ar} - |\Lambda|\omega_{ar}| < C_{ar}P$$

One-dimensional non-periodic systems

Theorem

Every one-dimensional lattice-gas model with finite-range interactions has at least one periodic ground-state configuration.

Thue-Morse sequences

substitutions

$0 \rightarrow 01$
$1 \rightarrow 10$

0

01

0110

01101001

0110100110010110

Let X be a Thue-Morse sequence, $X \in \{0,1\}^Z$

$$TM = closure(\{T_a X, a \in Z\})$$

$$\mu_{TM} = lim_{\Lambda \to Z} \frac{1}{|\Lambda|} \Sigma_{a \in \Lambda} \delta_{T_a} X$$

$$\lim_{k \to \infty} \frac{1}{k} \sum_{i=0}^{k-1} f(T^i(X)) = \int f d\mu_{TM}$$

(TM, T, μ_{TM}) is a uniquely ergodic dynamical system, Michael Keane, 1968

Characterizations of Thue-Morse sequences

Goal: looking for the minimal set of forbidden patterns

Gottschalk and Hedlung, 1964

TM is uniquely characterized by the absence of BBb,

where B is any word and b is its first character, 0 or 1

TM is uniquely characterized by the absence of infinitely many 4-point patterns
(Gardner, Radin, Miękisz, van Enter, 1989)

Theorem The following spin Hamiltonian has the Thue-Morse measure μ_{TM} as its unique ground state.

$$H = \sum_{j=-\infty}^{\infty} \sum_{p=0}^{\infty} \sum_{r=0}^{\infty} V(j,p,r) \qquad \sigma_i = \pm 1$$

$$= \sum_{j=-\infty}^{\infty} \sum_{p=0}^{\infty} \sum_{r=0}^{\infty} \exp[-(r+p)^2](\sigma_j + \sigma_{j+2^r})^2(\sigma_{j+(2p+1)2^r} + \sigma_{j+(2p+2)2^r})^2$$

Theorem (C. Gardner, JM, C. Radin, A. van Enter, 1989)

Thue-Morse sequences re uniquely characterized by the absence of 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 $(2p+1)2^r$, $r, p \geq 0$.

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 $0 \le \phi \le 2\pi$ 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 $a(n) = 1$.

Most homogeneous configurations

Definition 3. Let $X \in \{0,1\}^Z$ and $x_i \in Z$ be a position of a i-th 1 (a particle) in X. X is **most homogeneous** if there exists a sequence of natural numbers d_j such that $x_{i+j} - x_i \in \{d_j, d_j+1\}$ for every $i \in Z$ and $j \in N$.

Fibonacci sequences are most homogeneous

$$d_j = [j(2+\gamma)], \quad \gamma = \frac{2}{1+\sqrt{5}}, \quad [y] \; is \; an \; integer \; value \; of \; y$$

Forbidden distances between 1's = 1,4,9,12,17,22,25,30,…

We also forbid 000

and construct non-frustrated Hamiltonian with Fibonacci sequences as only ground-state configurations

van Enter, Koivusalo, Miękisz, J.Stat. Phys. 2020

Summary

Stability of non-periodic tilings

zero-temperature stability

Let μ be a unique non-periodic ground state of H.
Is μ a ground-state for H' = H + εH''
for any finite-range interaction H'' and a sufficiently small ε?

low-temperature stability

Does H have a non-periodic Gibbs state
which is a small perturbation of μ
at low temperature?

Fundamental Open Problem

Does there exist a non-periodic Gibbs measure which is
a small-temperature perturbation of a non-periodic ground state
of a lattice-gas model with translation-invariant finite-range interactions?

Thank you for your attention

Special thanks to

Grant NCN Harmonia

Mathematical models of quasicrystals

NARODOWE
CENTRUM
NAUKI