Aperiodic structures, notions of order and disorder

Shelomo I Ben-Abraham

Ben-Gurion University, Beer-Sheba, Israel

and

Alexander Quandt

University of Greifswald, Greifswald, Germany

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Outline

Motivation

Aperiodic heterostructures

Two-dimensional Prouhet-Thue-Morse

and paperfolding structures

Order and disorder

Symbolic complexity and entropy

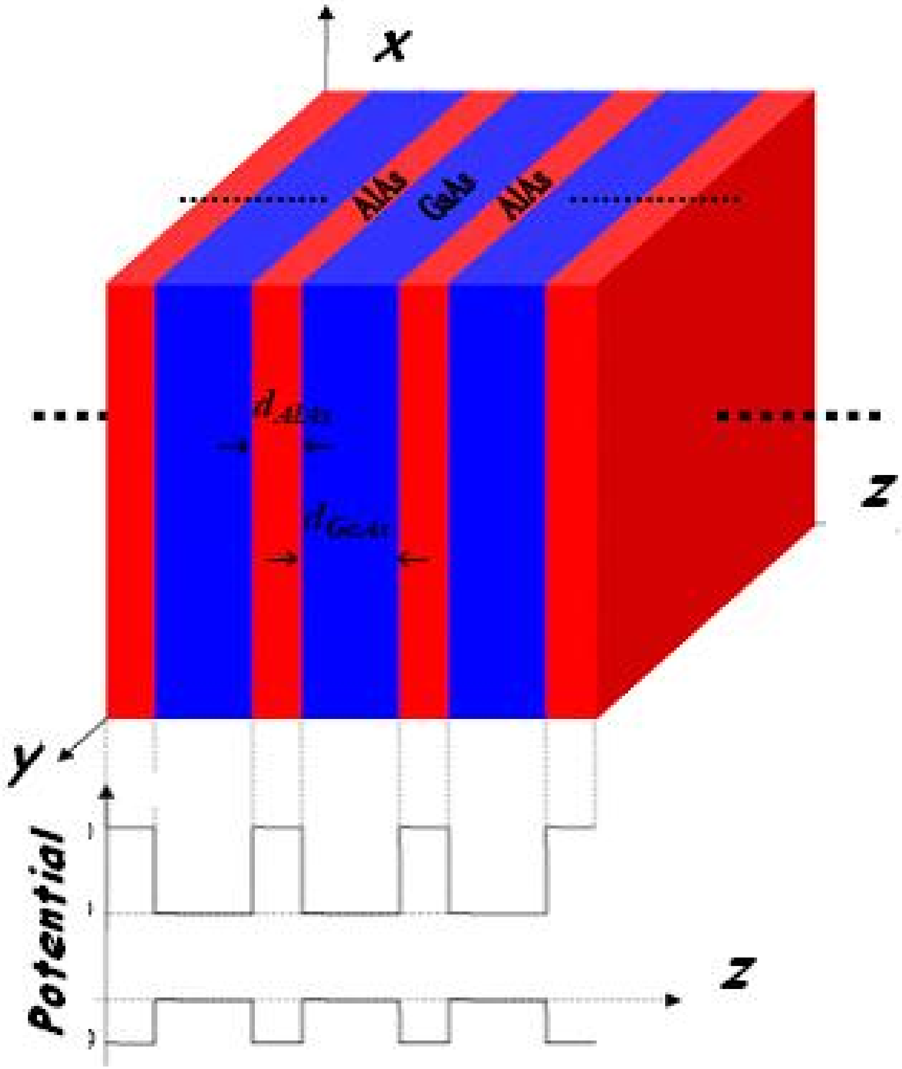
Motivation

Applications:

quasiregular (layered) heterostructures,
photonic and phononic metamaterials
(as optical and acoustical bandpassfilters
and much more)

Materials:
GaAs-AlGaAs,
other III-V and II-VI semiconductors,
Ge, Si, porous Si,
modulation by waves

GaAs-AlAs slab



How to produce such a structure?
MBE (Molecular Beam Epitaxy)

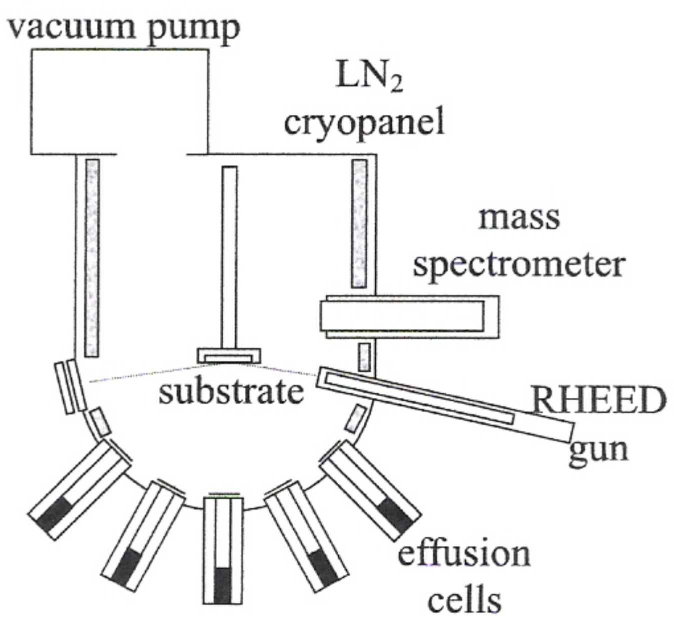
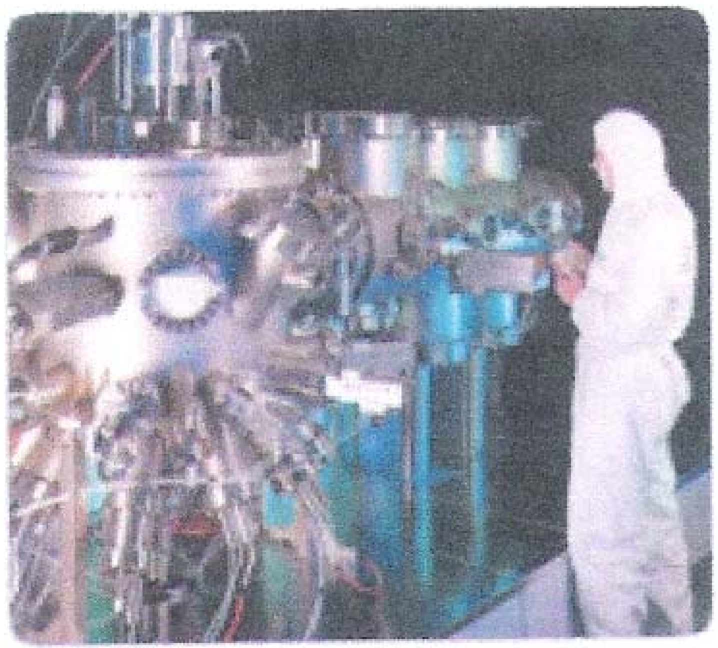


Fig. 1: A typical MBE system.



V90 molecular beam epitaxy (MBE) system

Sheer intellectual curiosity:

properties of multidimensional substitution systems; fundamental questions about determinism, order vs. disorder, complexity, entropy

What are we doing?

- Construct and study double-sided versions of Fibonacci (F), Prouhet-Thue-Morse(PTM), paperfolding (PF), period doubling (PD) and Golay-Rudin-Shapiro (GRS) sequences. Their spectral properties and complexities are all well known but not so for higher dimensions.

- Generalize to *n*D; follow

Barbé A., von Haeseler F., *Correlation and spectral properties of multidimensional Thue-Morse sequences*, Int. J. Bifurcation and Chaos 17 (2007) 1265-1303 but simplify.

The recursion equations for the 1D double-sided PTM sequence are

$$a(-2x) = a(x)\ ,$$
$$a(-2x+1) = -a(x)\ , \quad x \in \text{☪}\ ,$$
$$a(0) = -1\ , a(1) = 1\ .$$

For the 1D PF sequence we have

$$a(2x+1)=a(x),\ a(4x)=1,\ a(4x+2)=-1,\ x\geq 0$$
$$a(2x)=a(x),\ a(4x-1)=-1,\ a(4x-3)=1,\ \ x\leq 0$$
$$a(0)=1, \quad x \in \text{☪}\ ,$$

This can be readily generalized to nD.

For a start (and for a current experiment) we stay in 2D. Choose an expanding matrix $\boldsymbol{M}$, a shift vector $\boldsymbol{s} = (1,0)$ and an entry $\boldsymbol{x} \in$ ☪^{2} .

The recursion is

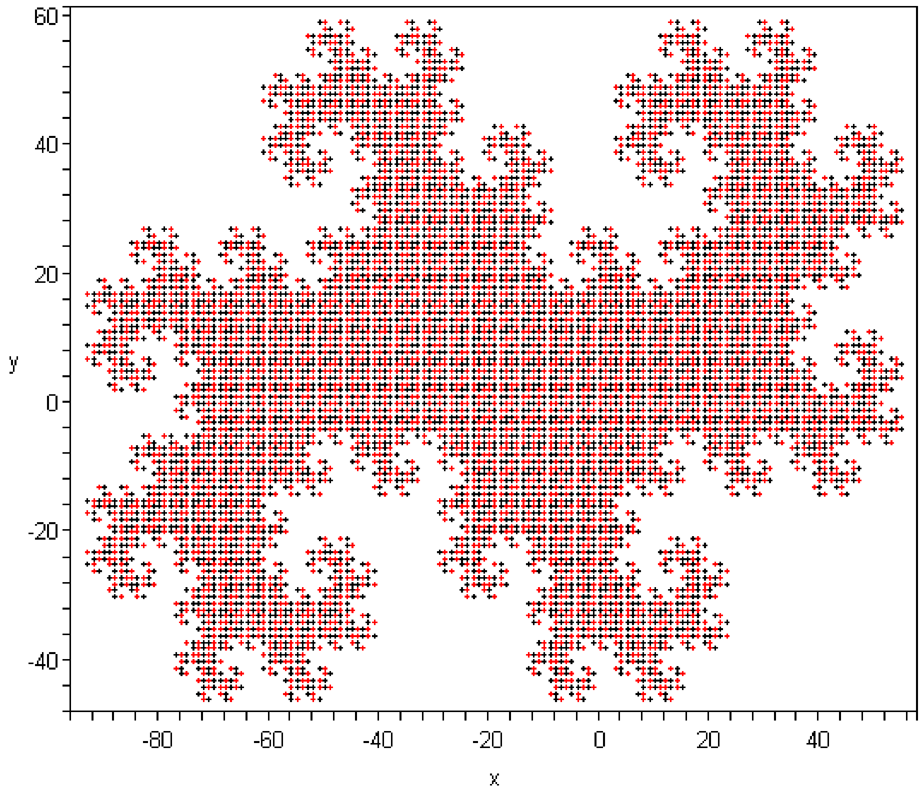
$$a(\boldsymbol{Mx}) = a(\boldsymbol{x}) \; ,$$

$$a(\boldsymbol{Mx}+\boldsymbol{s}) = -\,a(\boldsymbol{x}) \; , \quad \boldsymbol{x} \in \text{☪}^{2} \; ,$$

$$a(0,0) = -1 \; .$$

For the present example we choose

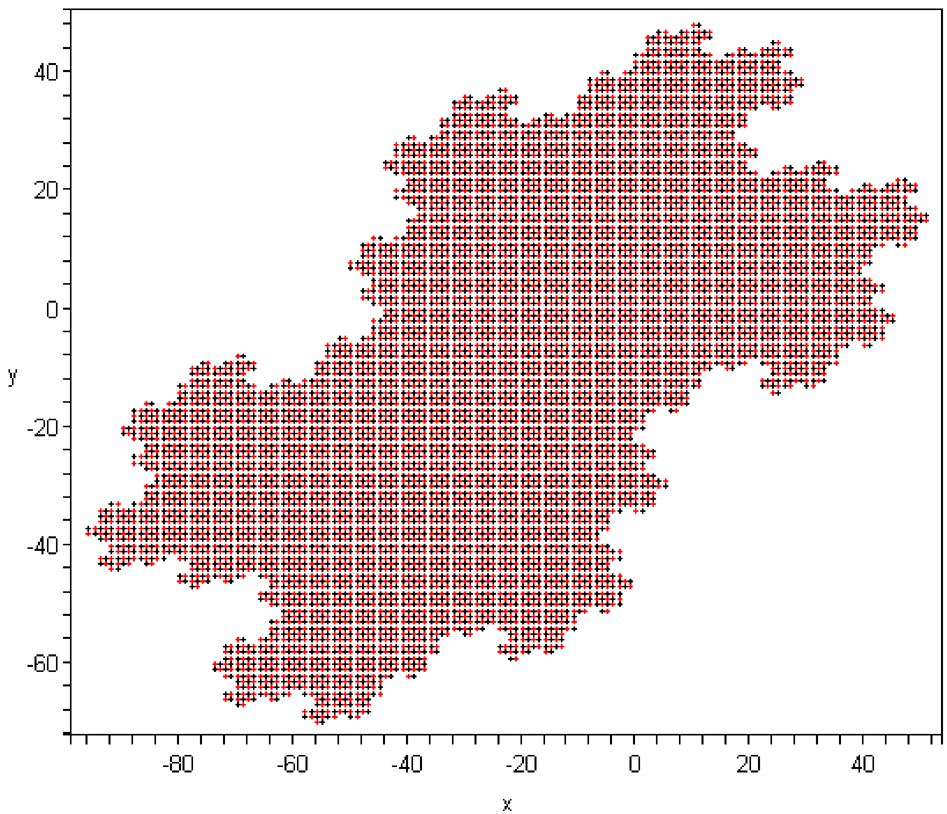
$$\boldsymbol{M} = \begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix} \; .$$



Patch of 2D PTM after 13 iterations containing $2^{13} = 8192$ points. This example is chiral and anorthotropic and has a fractal boundary.

To construct a *periodic* 2D PTM structure just change the matrix $\boldsymbol{M}$ to

$$\boldsymbol{M} = \begin{pmatrix} 0 & -2 \\ 1 & -1 \end{pmatrix}.$$



Patch of 2D PTM after 13 iterations containing $2^{13} = 8192$ points. This example is periodic and anorthotropic and has a fractal boundary.

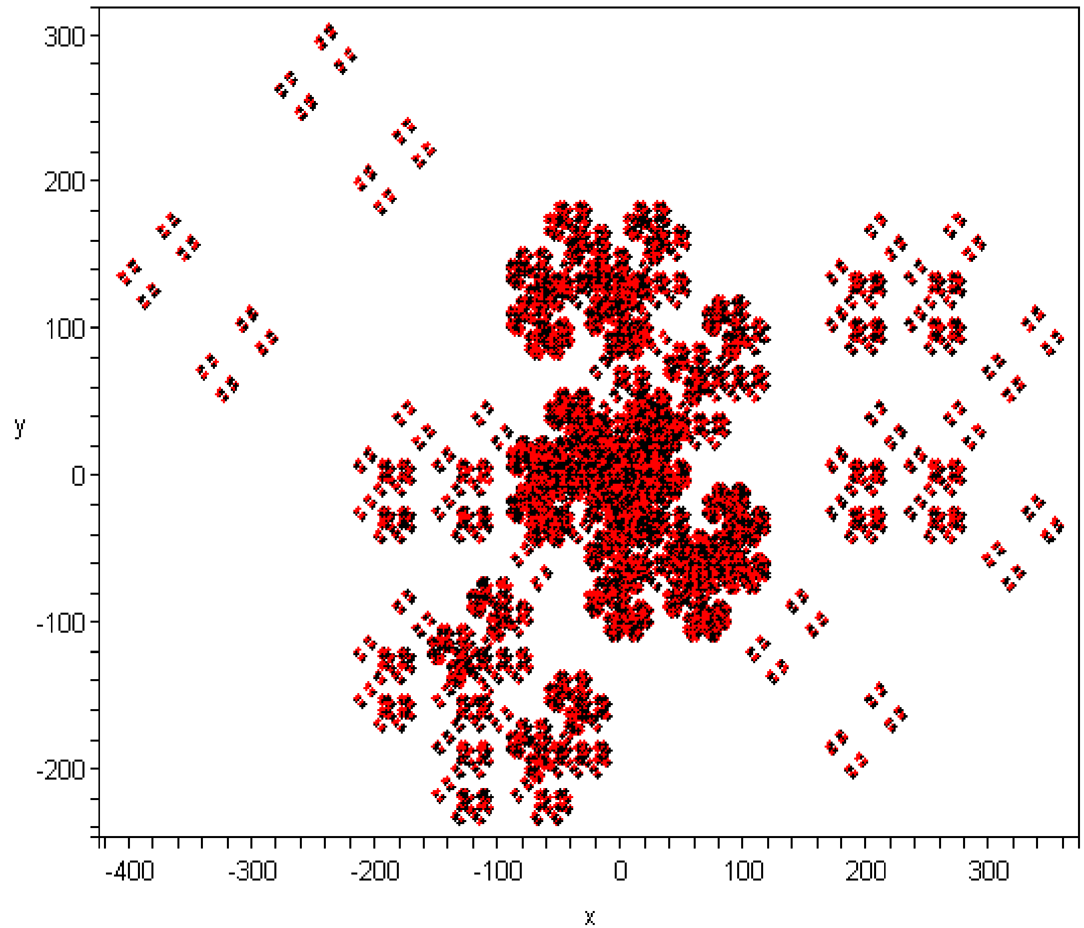
For the 2D paperfolding sequence the recursion is

$$a(\boldsymbol{Mx}+\boldsymbol{s}) = a(\boldsymbol{x})\,,\; a(\boldsymbol{M}^2\boldsymbol{x}) = 1\,,\; a(\boldsymbol{M}^2\boldsymbol{x}+\boldsymbol{Mx}) = -1\,,$$

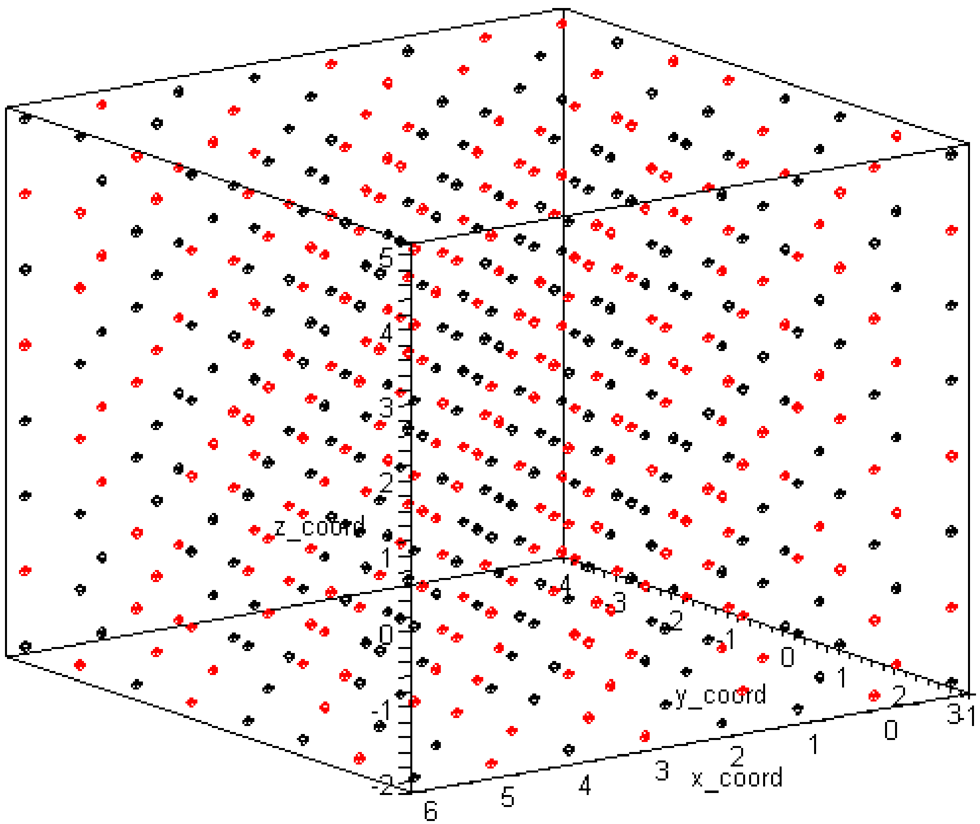
$$a(0,0) = 1\,,\quad \boldsymbol{x} \in \mathbb{Z}^2\,,$$

with the same matrix $\boldsymbol{M}$:

$$\boldsymbol{M} = \begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix} \;.$$



Patch of 2D PF after 9 iterations containing 19683 points. This example is anorthotropic and has an extremely fractal boundary.



A 3D example

“order ↔ disorder”

“cold ↔ hot”

Intuitive but undefined, subjective, context dependent

Quantify “cold ↔ hot” by temperature (energy, frequency)

Quantify “order ↔ disorder” by entropy (negentropy = information)

??? determinism ⇔ order ???

Entropy is insufficient to characterize such structures. More revealing and detailed is symbolic complexity: a function $p_S(n)$ counting the number of words of length n in a sequence S:

$$p_{1010\ldots}(n) = 2 \text{ for all } n,$$

$$p_{\text{Fibonacci}}(n) = n+1 \text{ for all } n,$$

$$p_{\text{RS}}(n) = 8(n-1) \text{ for } n \geq 8,$$

!!! $p_{\text{Champernowne}}(n) = 2^n$ for all n !!!

Entropy:

$$H(S) := \lim_{n\to\infty} \frac{\ln p_{S(n)}}{n}$$

Eventually we computed the symbolic complexity of our examples. We started with *lattice animals (polyominoes)* and learned a few things, such as: the generic example of PTM is *chiral* and *anorthotropic*. Yet the numeric effort is disproportional. So we compromised and computed the *rectangle complexity*. To gain rapid insight we focused on *lines,* i.e. *rows* and *columns*. This explicitly confirmed the chirality and anorthotropy. The recursion makes the boundary *fractal*. The complexity is approximately quadratic, polynomial at most; hence the entropy is zero. The PF example is similar but it is not chiral and its complexity is roughly linear.

Symbolic complexity of 2D PTM						Symbolic complexity of 2D PF			
N	$p_r(N,1)$	$p_c(1,N)$	$p_\ell(N)$	N^2		$p_r(N,1)$	$p_c(1,N)$	$p_\ell(N)$	$8(N-2)$
1	2*	2*	2*	1		2*	2*	2*	-8
2	4	4	8	4		4	4	8	0
3	6	6	12	9		8	8	16	8
4	8	10	18	16		11	11	22	16
5	10	14	24	25		15	15	30	24
6	14	20	34	36		19	19	38	32
7	18	26	44	49		23	23	46	40
8	24	34	58	64		26	26	52	48
9	28	42	70	81		30	30	60	56
10	34	52	86	100		34	34	68	64
11	40	70	110	121		38	38	76	72
12	46	90	136	144		42	42	84	80
13	52	108	160	169		46	46	92	88
14	60	130	190	196		50	50	100	96
15	68	156	224	225		53	53	106	104
16	76	186	262	256		56	56	112	112
17	84	208	292	289		60	60	120	120
18	94	236	330	324		64	64	128	128
19	104	26	368	361		68	68	136	136
20	122	292	414	400		72	72	144	144

*) The entries for $N = 1$ are exceptional since rows and columns are the same: (1, 1).

Conclusions and outlook

The complexity of 2D PTM is at most polynomial, probably so for nD ($n > 2$), hence the entropy vanishes: $H=0$.

The complexity of 2D PF is roughly linear, it seems to satisfy $p=8(n-8)$ (needs proof!); the entropy vanishes: $H=0$.

We proceed to other instances of PTM and PF, other 2D sequences, to 3D etc.

Challenges

Find (define?) canonical prototypes for these 2D (nD) sequences.

Find formulas for the 2D (nD?) complexities.

When is the entropy of a deterministic structure zero? Is entropy a measure of randomness? Champernowne is a counterexample!

A vexing puzzle!

감사합니다！

谢谢！

Gracias!

Obrigado!

Thank you !

Merci!

Grazie!

תודה!

شكراً!

Спасибо!

Danke!

Ευχαριστω!

ありがとう！