Aperiodic structures, notions of order and disorder

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KIAS workshop:
The Mathematics of Aperiodic Order
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Outline

Motivation
Aperiodic heterostructures
Two-dimensional Prouhet-Thue-Morse and paperfolding structures
Order and disorder
Symbolic complexity and entropy
Some speculations
Motivation

Applications:
quasiregular (layered) heterostructures, photonic and phononic metamaterials (as optical and acoustical bandpass filters 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.
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.

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

\[
a(-2x) = a(x) ,
\]
\[
a(-2x + 1) = - a(x) , \quad x \in \mathbb{Z} ,
\]
\[
a(0) = -1 , \quad a(1) = 1 .
\]

For the 1D PF sequence we have

\[
a(2x+1) = a(x) , \quad a(4x) = 1 , \quad a(4x+2) = -1 , \quad x \geq 0
\]
\[
a(2x) = a(x) , \quad a(4x-1) = -1 , \quad a(4x-3) = 1 , \quad x \leq 0
\]
\[
a(0) = 1 , \quad x \in \mathbb{Z} ,
\]

This can be readily generalized to \(nD\).
For a start (and for a current experiment) we stay in 2D. Choose an expanding matrix $M$, a shift vector $s = (1,0)$ and an entry $x \in \mathbb{Z}^2$.

The recursion is

\[
a(Mx) = a(x) ,
\]

\[
a(Mx + s) = -a(x) , \quad x \in \mathbb{Z}^2 ,
\]

\[
a(0,0) = -1 .
\]

For the present example of PTM we choose

\[
M = \begin{pmatrix}
-1 & -1 \\
1 & -1
\end{pmatrix} .
\]
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 $M$ to

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

\[ a(Mx + s) = a(x) \, , \, a(M^2x) = 1 \, , \, a(M^2x + Mx) = -1 \, , \]
\[ a(0, 0) = 1 \, , \, x \in \mathbb{Z}^2 \, , \]

with the same matrix \( M \) :

\[
M = \begin{pmatrix}
-1 & -1 \\
1 & -1
\end{pmatrix}.
\]
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 $S$:

- $p_{1010\ldots}(n) = 2$ for all $n$,
- $p_{\text{Fibonacci}}(n) = n + 1$ for all $n$,
- $p_{\text{PF}}(n) = 4n$ for $n \geq 7$,
- $p_{\text{GRS}}(n) = 8(n - 1)$ for $n \geq 8$,
- $p_{\text{Champernowne}}(n) = 2^n$ for all $n$.

Topological 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 2D PTM 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

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<th>$p_r(N, 1)$</th>
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Symbolic complexity of 2D PF

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*) Entries for $N = 1$ are exceptional since rows and columns are the same: $(1, 1)$. 
Some speculations and afterthoughts:

- The BvH algorithm produces, depending on $M$, infinitely many instances of a given structure. Can we define a canonical prototype?
- Can we define a single number characteristic for the complexity of a given (instance of a) structure $S$? Exponent of $p_S(N)$ as a power law?
- What can we learn from deterministic chaos? Approximate or sample entropy?
- How to tell deterministic irregularity/normality from stochasticity?
Conclusions and outlook

The complexity of 2D PTM is at most polynomial, Most probably so for $nD$ ($n > 2$), hence the entropy vanishes: $H = 0$.
The complexity of 2D PF is roughly linear, it seems to satisfy $p_{PF}(N) = 8(N - 2)$ (needs proof!); the entropy vanishes: $H = 0$.

We proceed to other instances of PTM and PF, other 2D sequences, to 3D etc.
We develop alternative algorithms.
We try to find a concise characteristic of nonuniformity for a given structure.
Find formulae for the 2D ($nD$?) complexities.
감사합니다！
谢谢！
Gracias!
Thank you!
Obrigado!
Merci!
Grazie!
شكراً!
Cnacubo!
Danke!
Евхаристо!
ありがとう！
TM 60 mm x 60 mm; grid separation = 1 mm; hole $\varnothing = 0.4$ mm
Oy polarization

Intensity

THz

0.13
0.197
0.24
0.34
0.376
Gracias!

Thank you

Grazie!

Obrigado!

Merci!

สวน!

חודה!

Danke!

Cnacubo!

Ευχαριστώ!
Double-sided sequences

Fibonacci

∅

b b

a a

ba ab

aba aba

baaba abaab

ababaabaaba abaabababaabaabaabab
2D generalization
2D Prouhet-Thue-Morse (full)
2D Prouhet-Thue-Morse (cutout)
2D Prouhet-Thue-Morse Fourier transform
TM 60 mm x 60 mm;
grid separation = 1 mm; hole \( \varnothing = 0.4 \) mm
Paper folding:

\[ S(0) = a, \quad S(n + 1) = S(n) a F\left( S(n) \right), \]

\[ F: \tilde{S}(a, b) \rightarrow \tilde{S}(b, a) \]

reverse and interchange

\[ S(3) = aabaabbaaabbabbb \]

Period doubling:

\[ a \rightarrow ab, \quad b \rightarrow aa, \quad S(0) = b \]

\[ S(4) = abaaababababaaababab \]
Interesting: Miroslav Kolář’s group, e.g.:

M.Kolář, M.K. Ali, Franco Nori,
*Generalized Thue-Morse chains and their physical properties,*
PRB 43 (1991) 1034-1047
Paper folding:

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ありがとう！