Course IMSc Chennai, India

January-March 2017

Enumerative and algebraic combinatorics,
a bijective approach:

commutations and heaps of pieces

(with interactions in physics, mathematics and computer science)

Monday and Thursday 14h-15h30

www.xavierviennot.org/coursIMSc2017

IMSc
January-March 2017

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Chapter 7

Heaps in statistical mechanics (1)

IMSc, Chennai

2 March 2017

a few words about

statistical mechanics .....

phase transition
critical phenomena

from local interactions
→ global behaviour

exactly
solved
models

Ising
model

Baxter
book (1982)

Onsager (1944)

Statistical physics

$$F(T) \cong \frac{1}{(T - T_c)^{\alpha}}$$

critical exponent

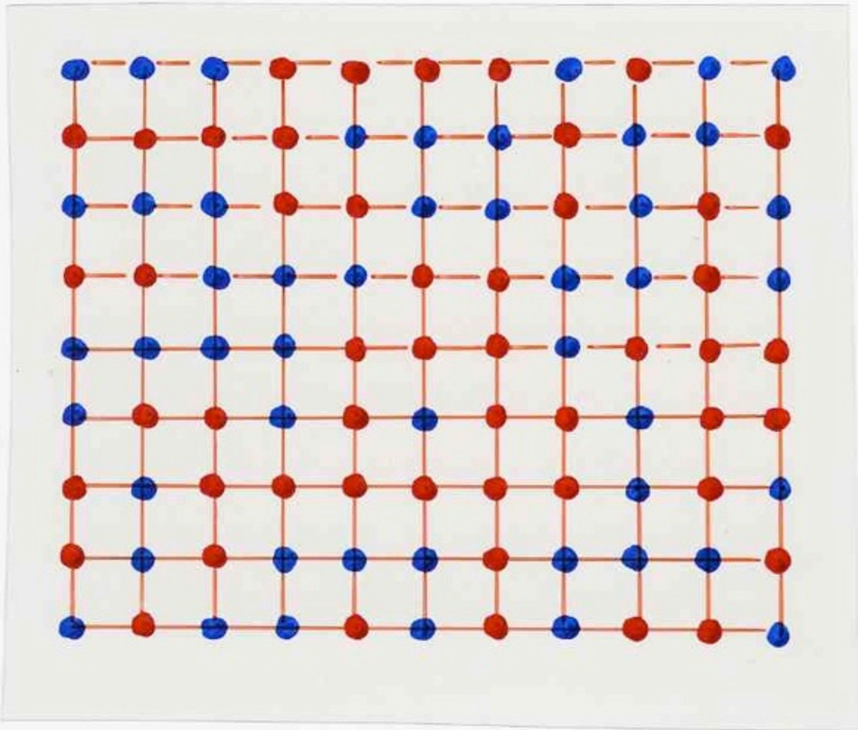
temperature

thermodynamic function

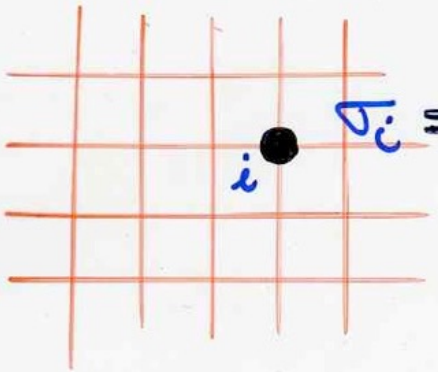
critical temperature

example 1:

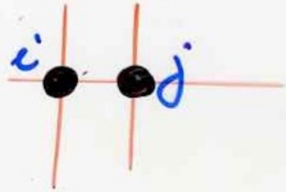
the Ising model



Ising model



$\sigma_i = \pm 1$



interaction

$$E_{ij} = J_{ij}\,\sigma_i\sigma_j$$

total energy

σ configuration

$$E_\sigma = -J\sum_{i,j} \sigma_i\sigma_j - I\sum_i \sigma_i$$

adjacent

external field

$J > 0$ ferromagnétisme

$J < 0$ (anti- - - - - - .)

Partition function

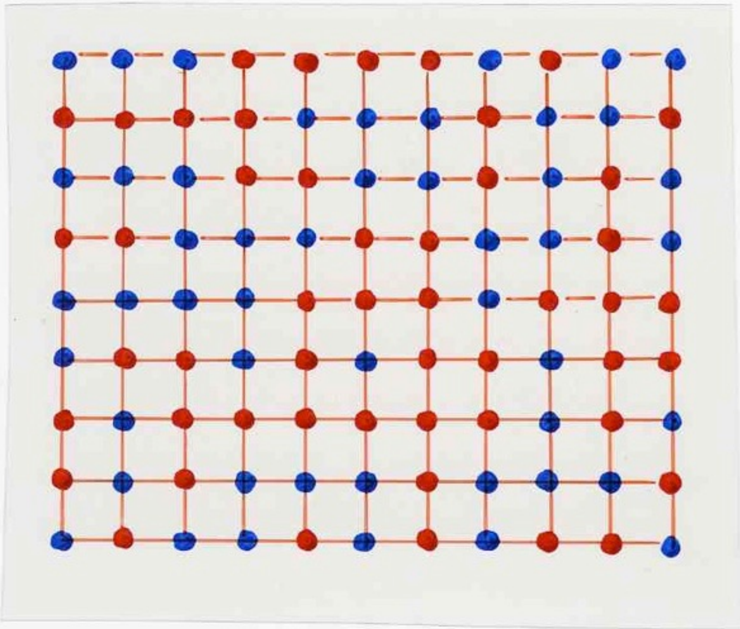
$$Z_L = \sum_{\sigma} \exp\left(-E_\sigma / kT\right)$$

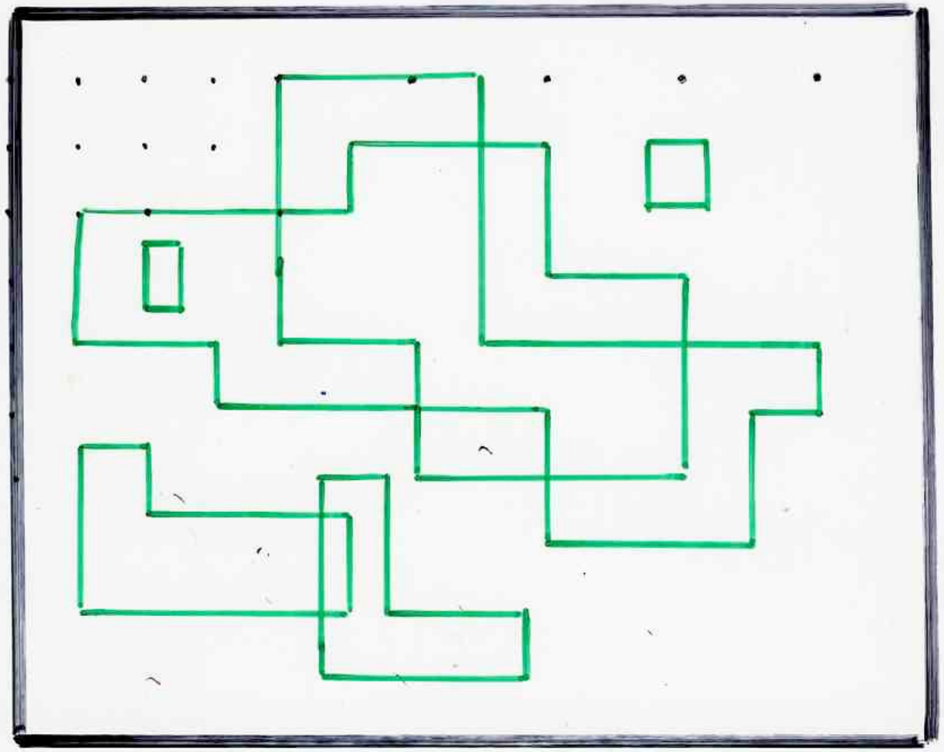
k Boltzmann constant
T temperature

$$Z_L = (\mathrm{ch}\, H)^N 2^N \, Cl_L(\mathrm{th}\, H)$$

generating function for closed subgraphs

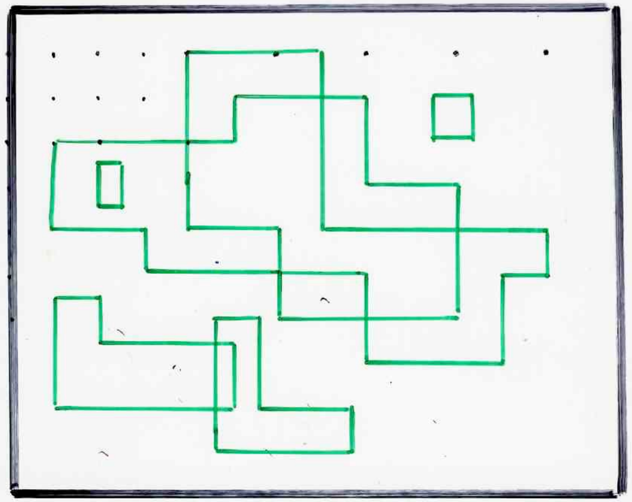
(enumerated by total number of edges)





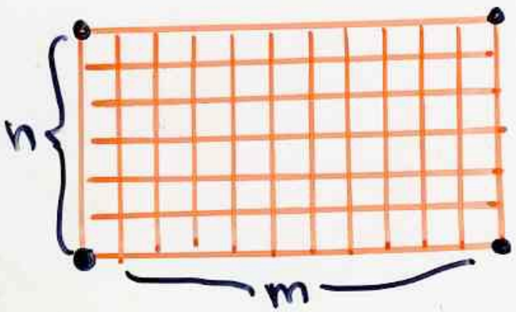
"closed" graph

Ising model



"closed" graph

Ising model

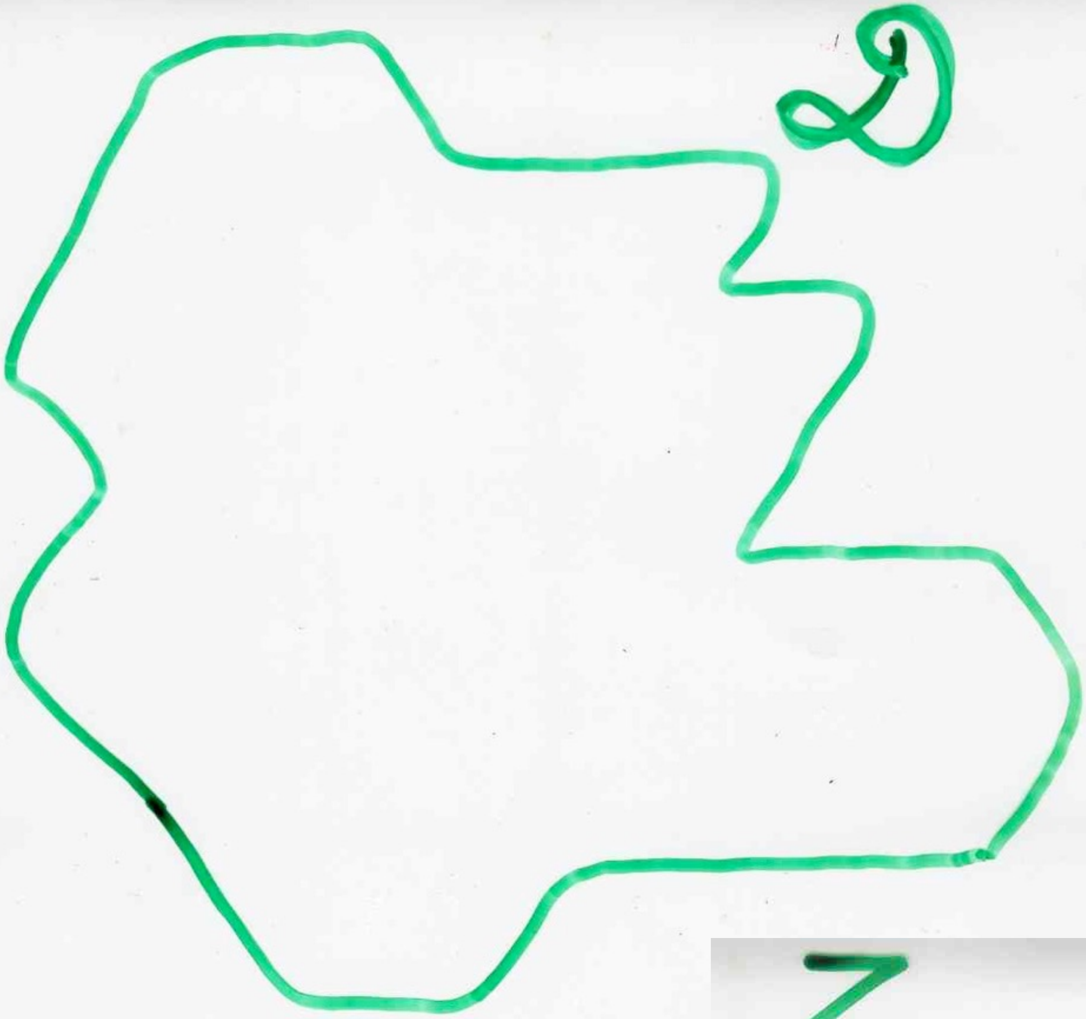


thermodynamic limit

"$N \to \infty$"

$$N = nm$$

$$Z = \lim_{``N \to \infty"} Z_{n,m}^{1/N} .$$

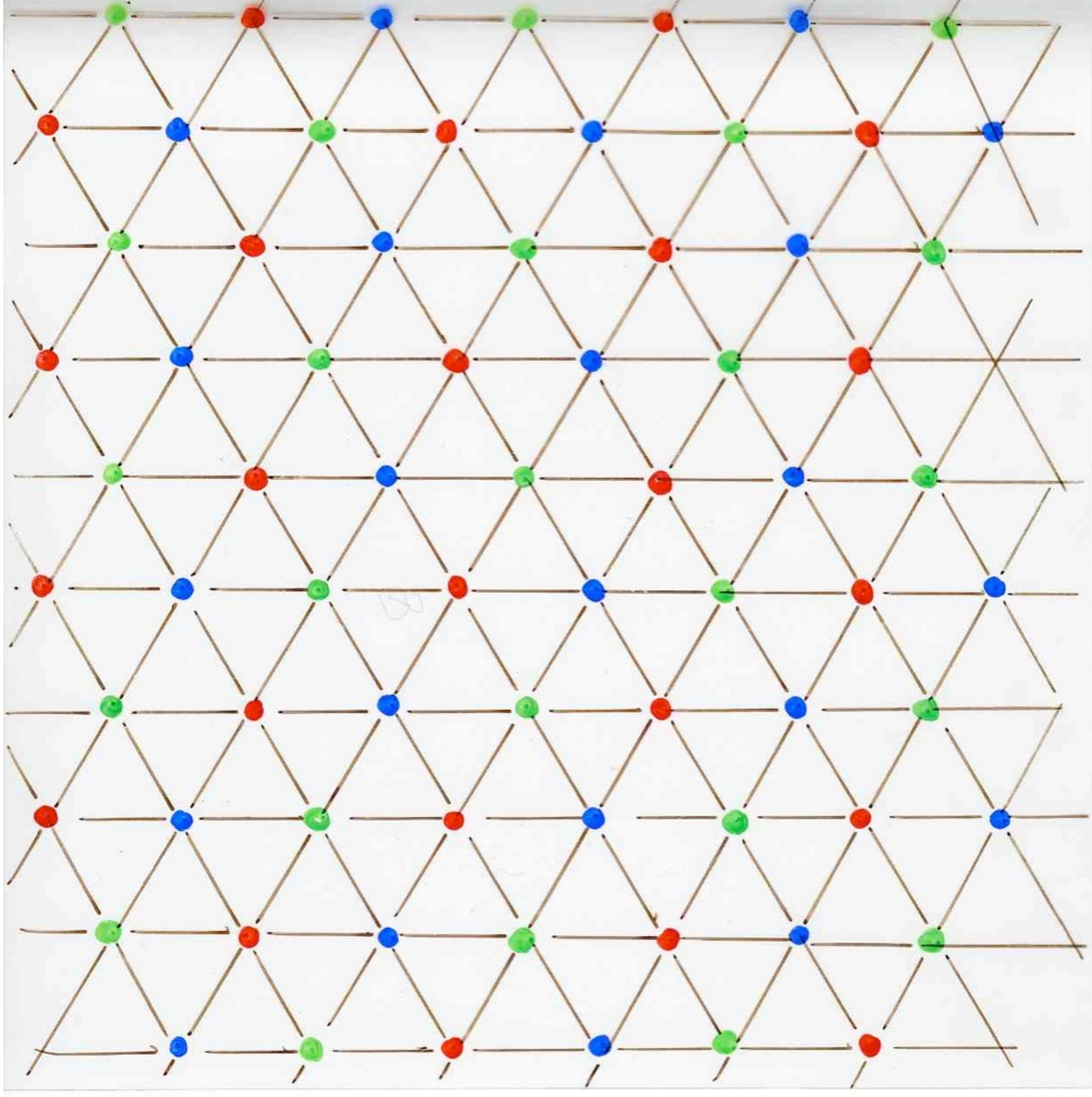


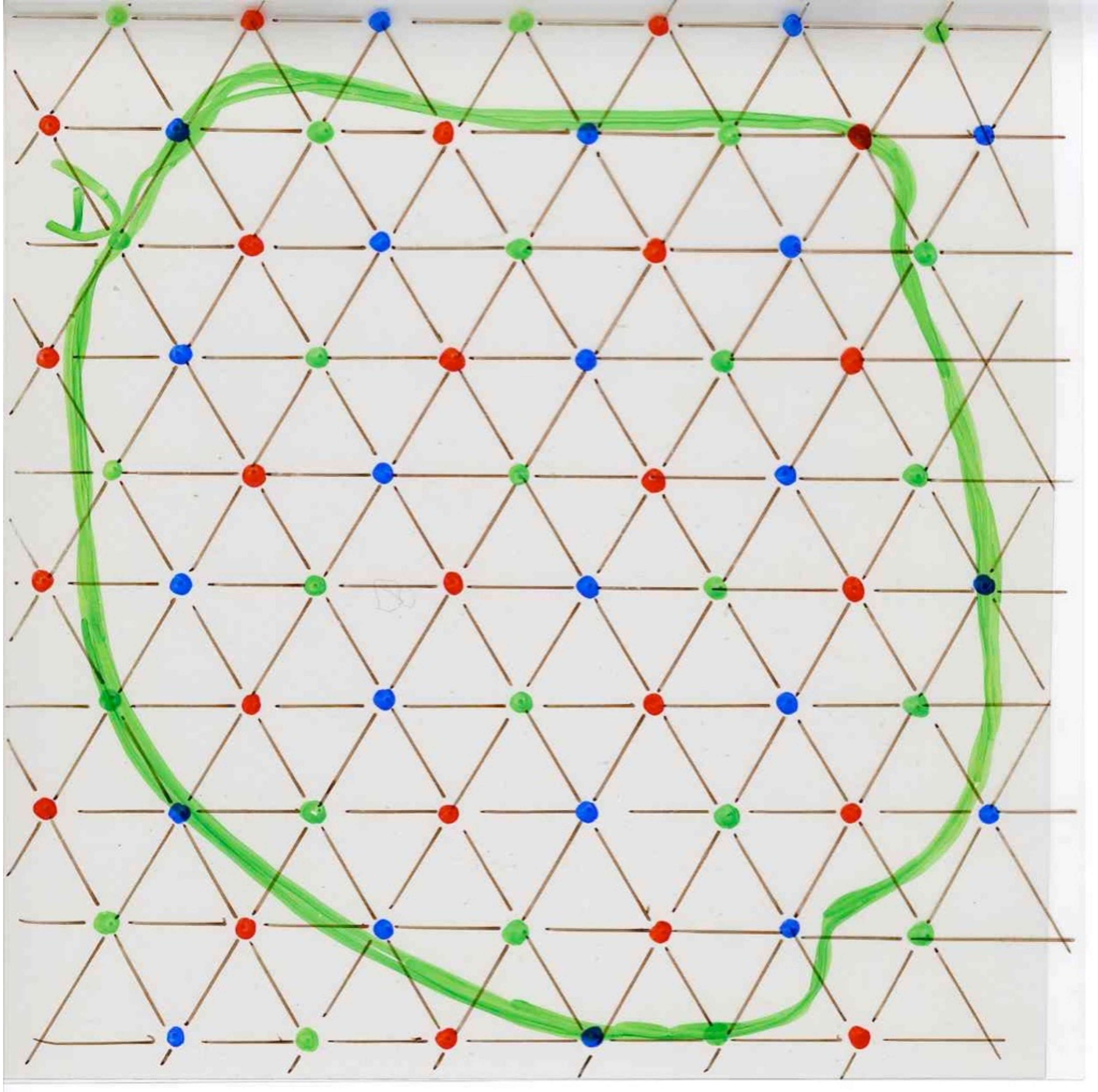
$Z_{\mathcal{D}}$ partition function

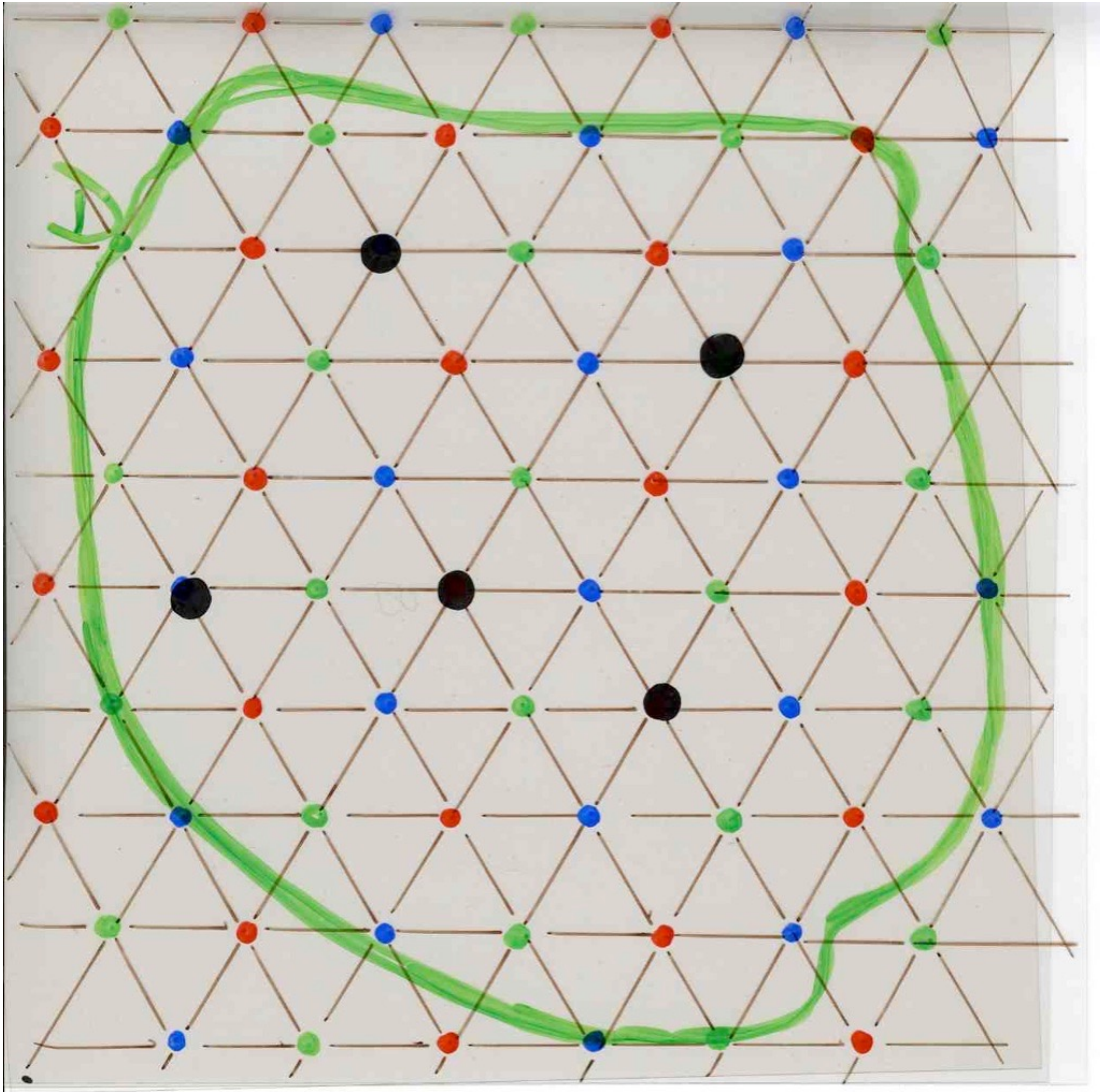
$$Z = \lim_{``\mathcal{D} \to \infty"} Z_{\mathcal{D}}^{1/N}$$

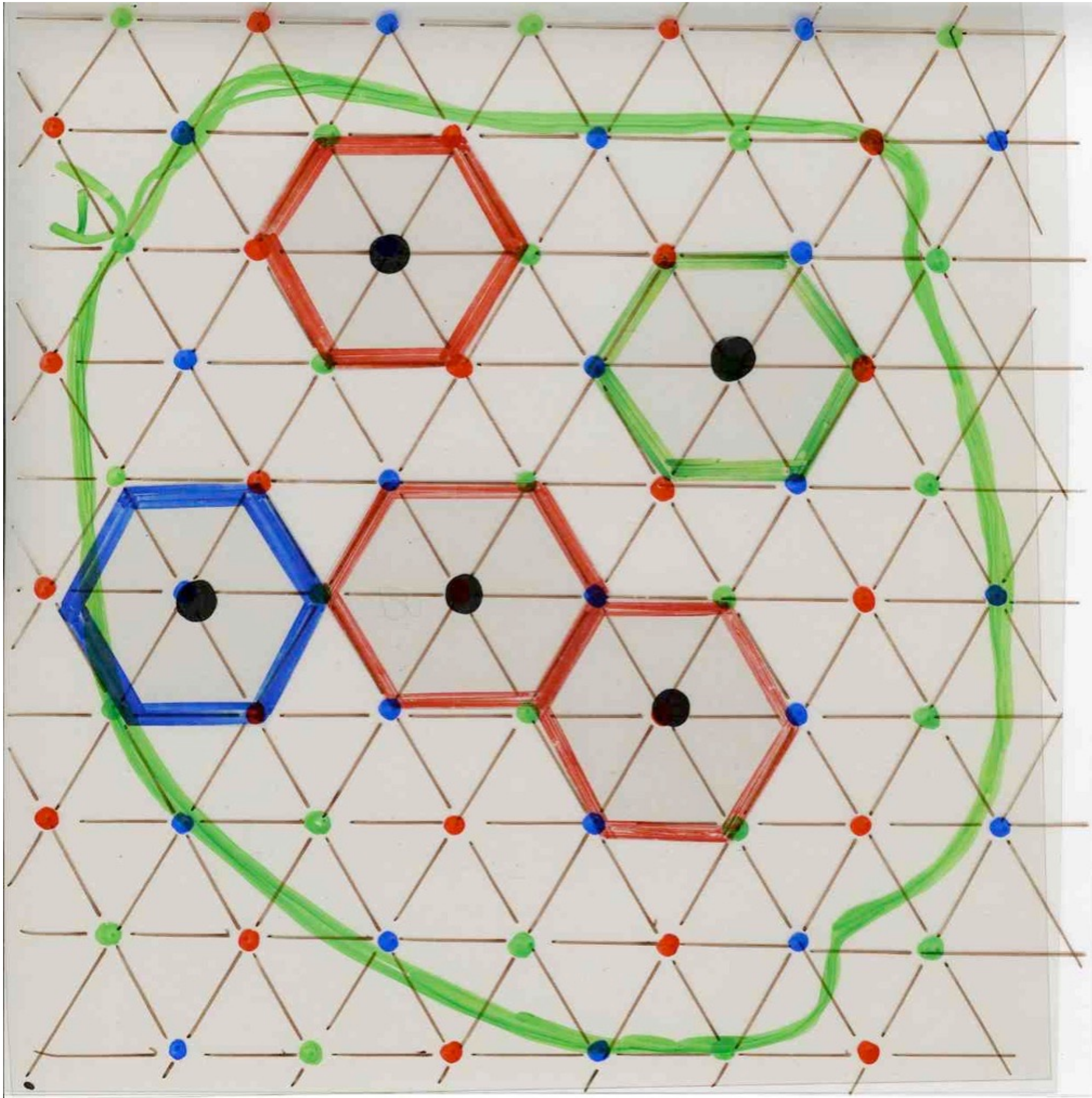
example 2:

gas model









partition function

$$Z_D(t) = \sum_{n \geq 0} a_{n,D}\, t^n$$

$$Z(t) = \lim_{\text{"}D \to \infty\text{"}} \left(Z_D(t) \right)^{1/|D|}$$

thermodynamic limit

Hard Hexagons

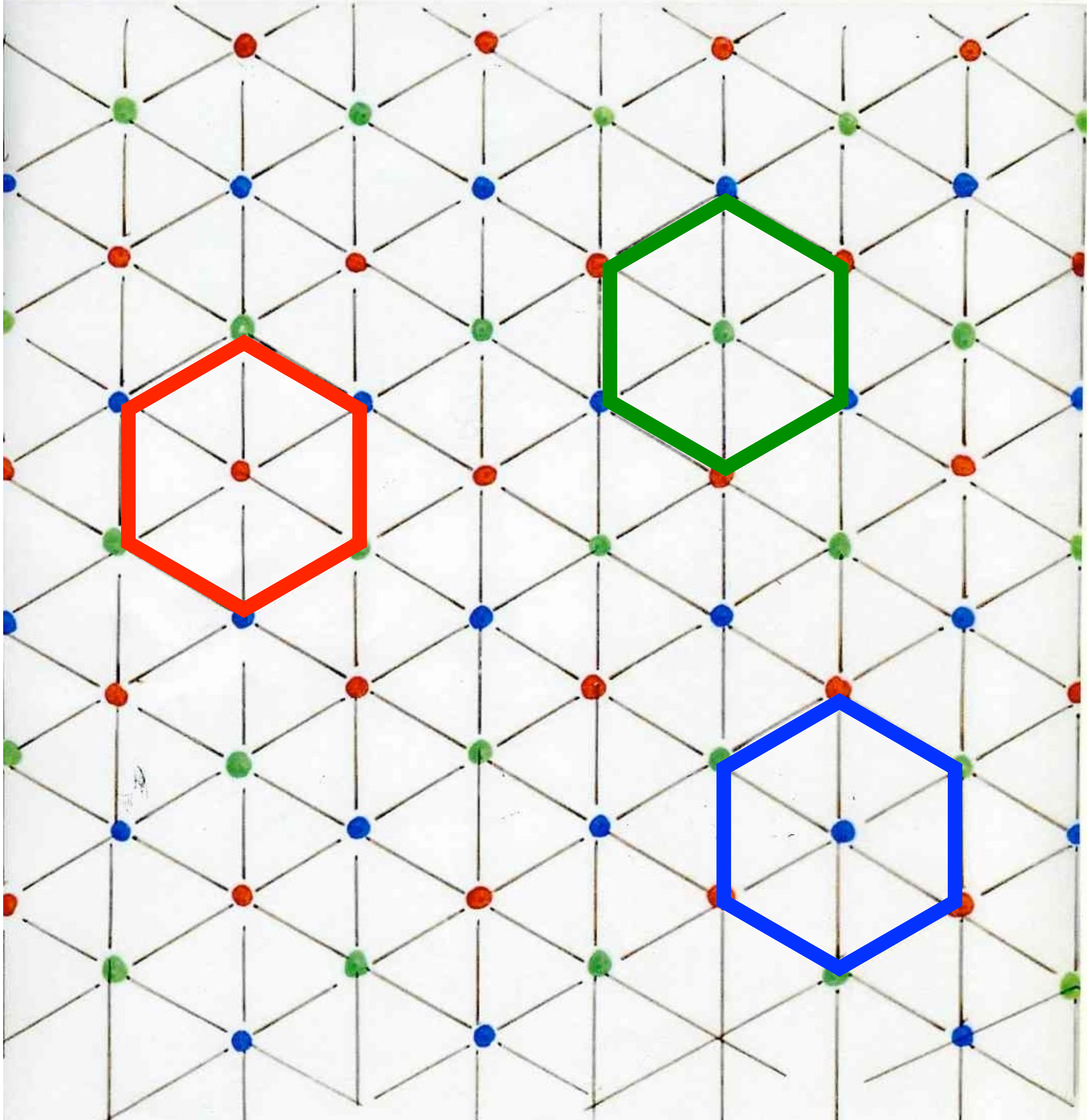
Baxter

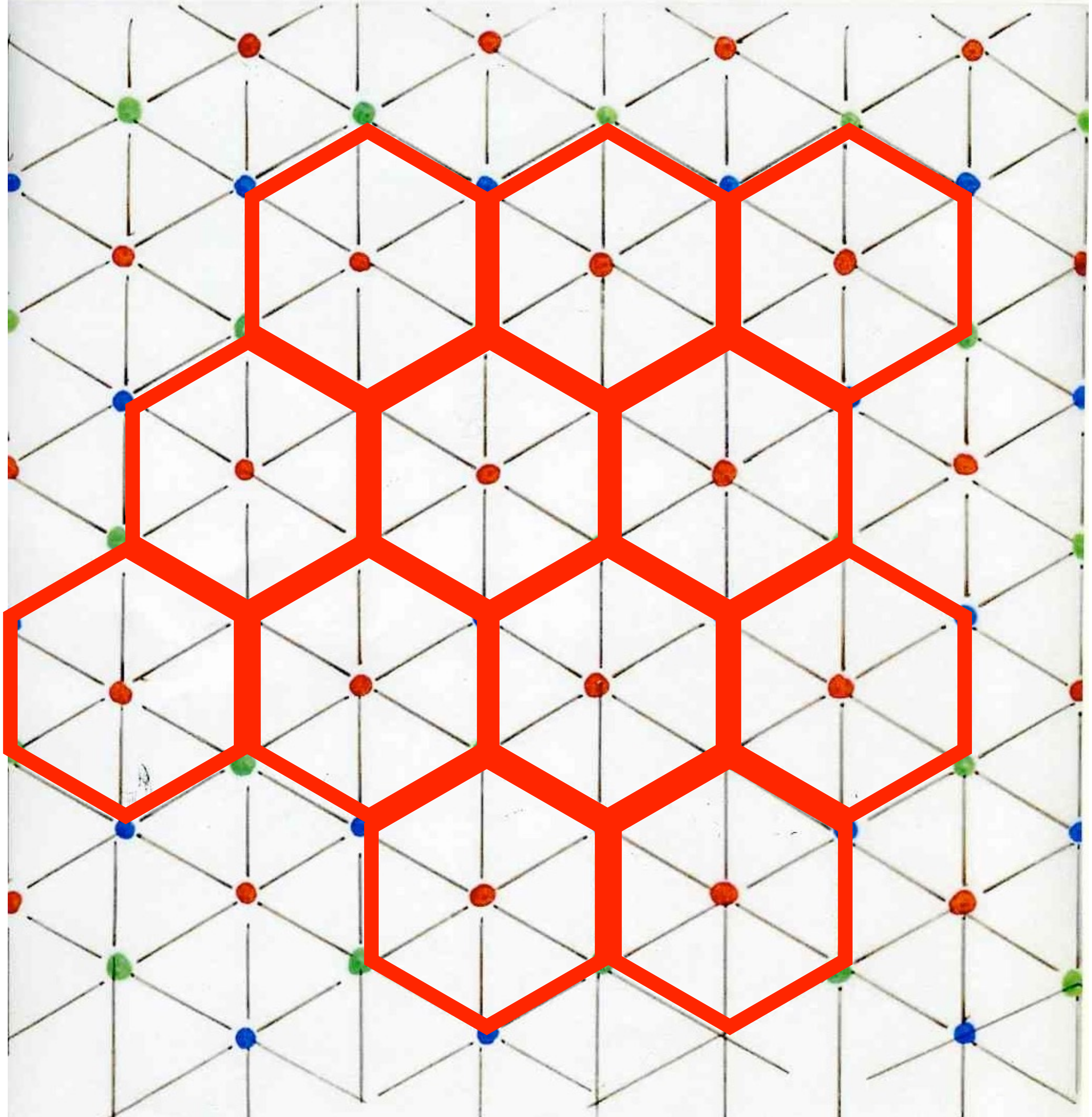
1980

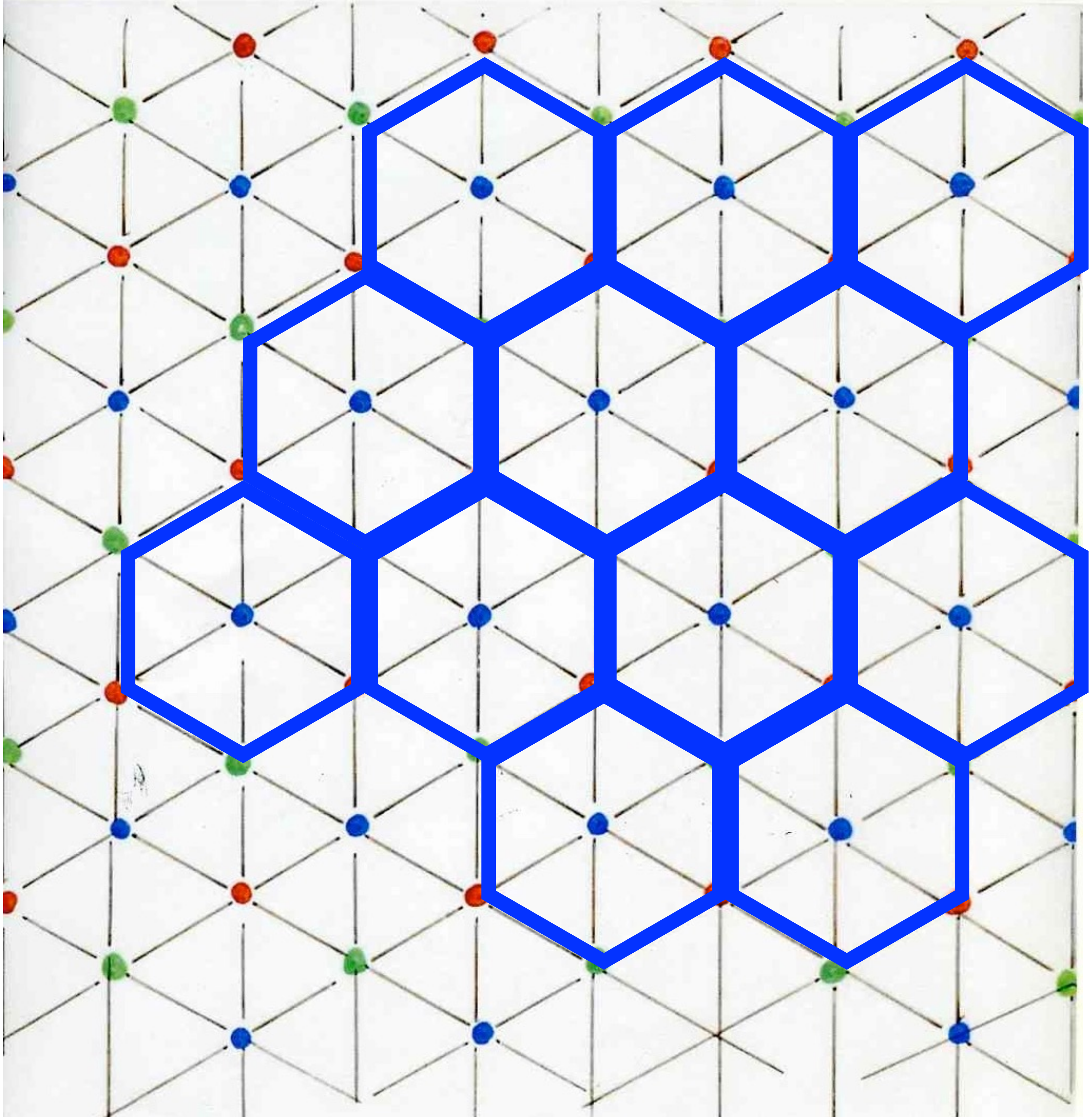
1982

gas model

with "hardcore interactions"



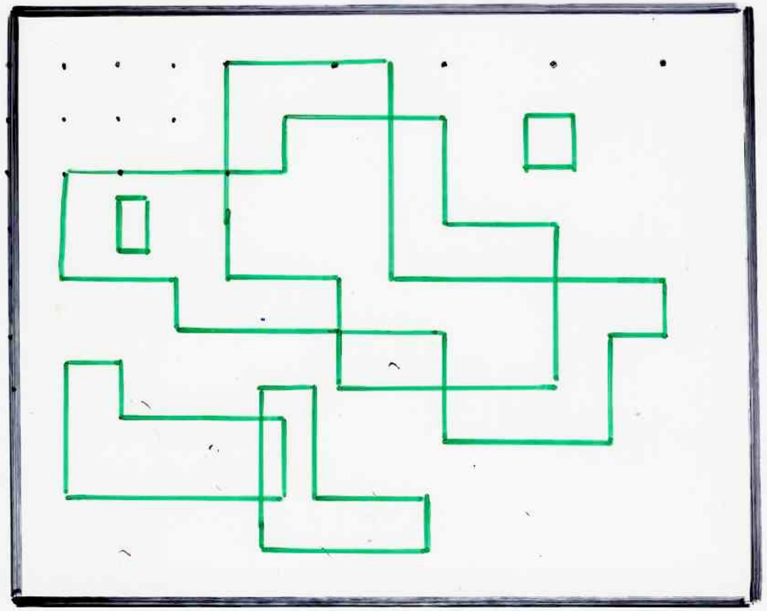




statistical mechanics

and

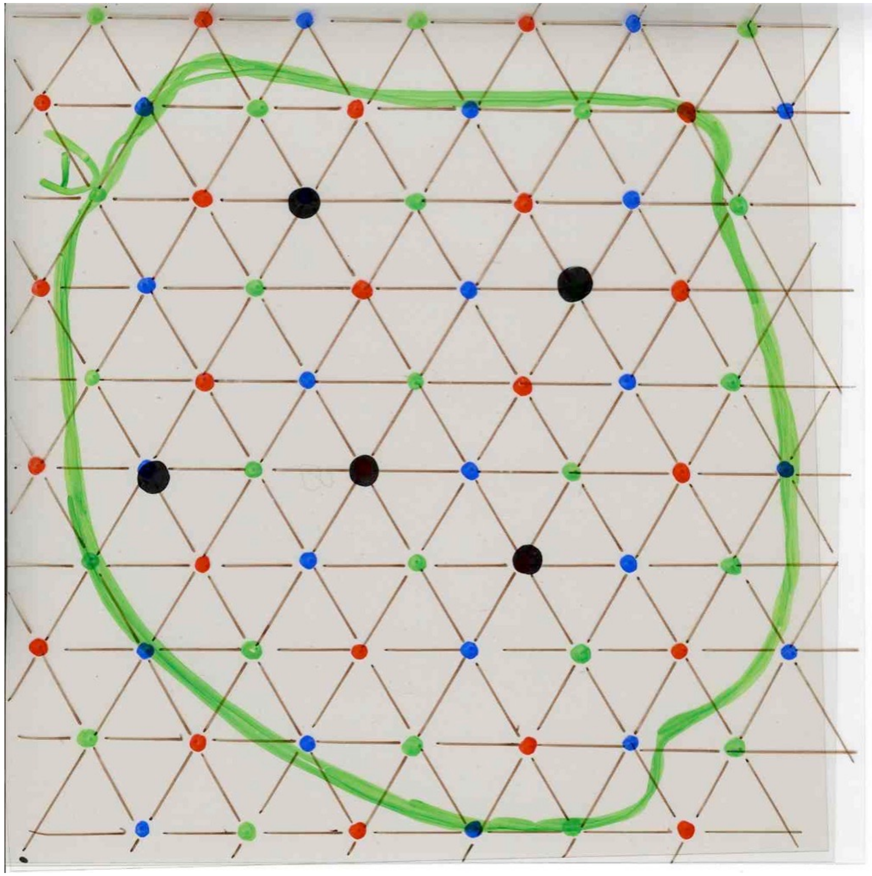
combinatorics



"closed" graph Ising model

before the

thermodynamic limit



Statistical physics

$$F(T) \cong \frac{1}{(T - T_c)^{\alpha}}$$

thermodynamic function

temperature

critical temperature

critical exponent

Polyominoes
animals
heaps

and physics

$$F(T) = \sum_{n\geq 0} a_n T^n$$

partition function

$$F(T) \simeq \frac{1}{(T - T_c)^{\alpha}}$$

critical exponents

$$a_n \sim \mu^n n^{-\theta}$$

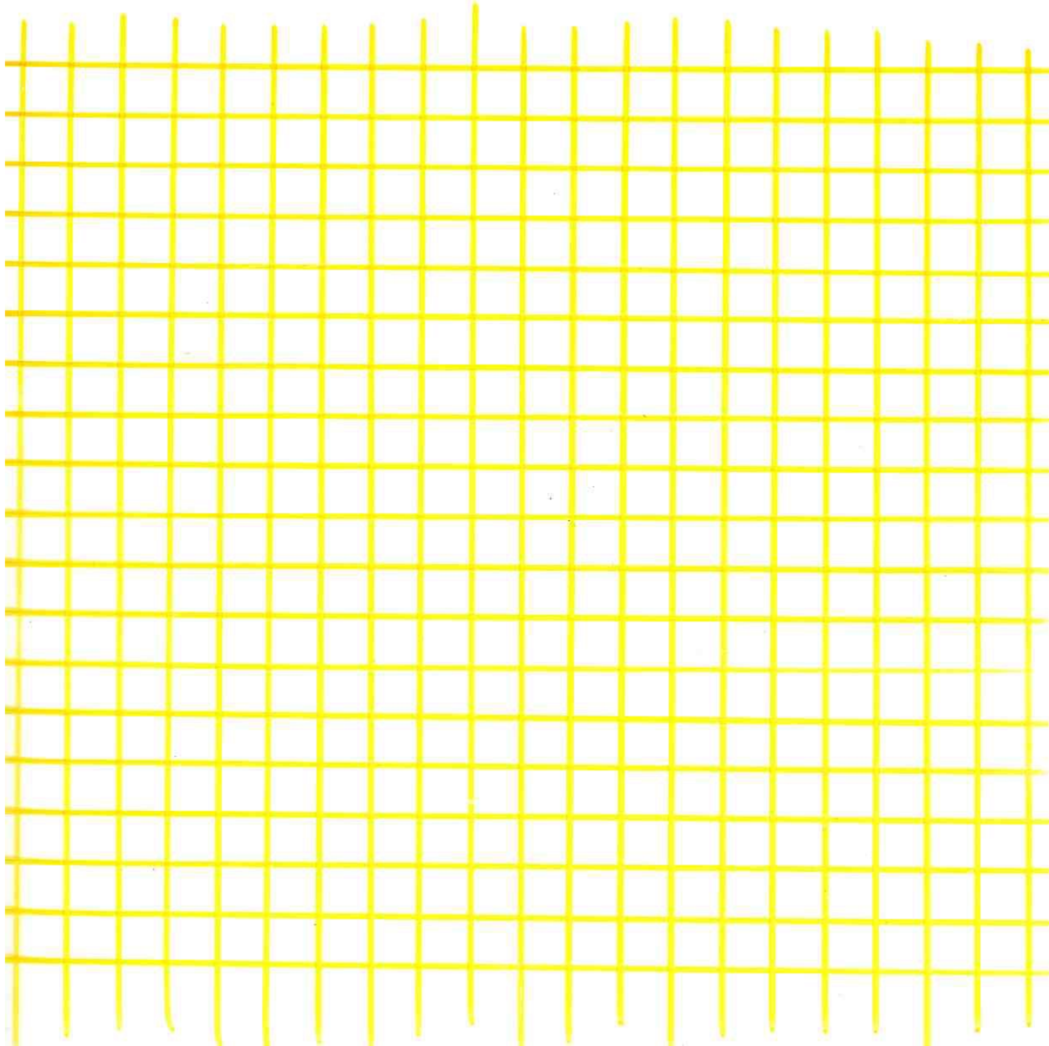
after the

thermodynamic limit

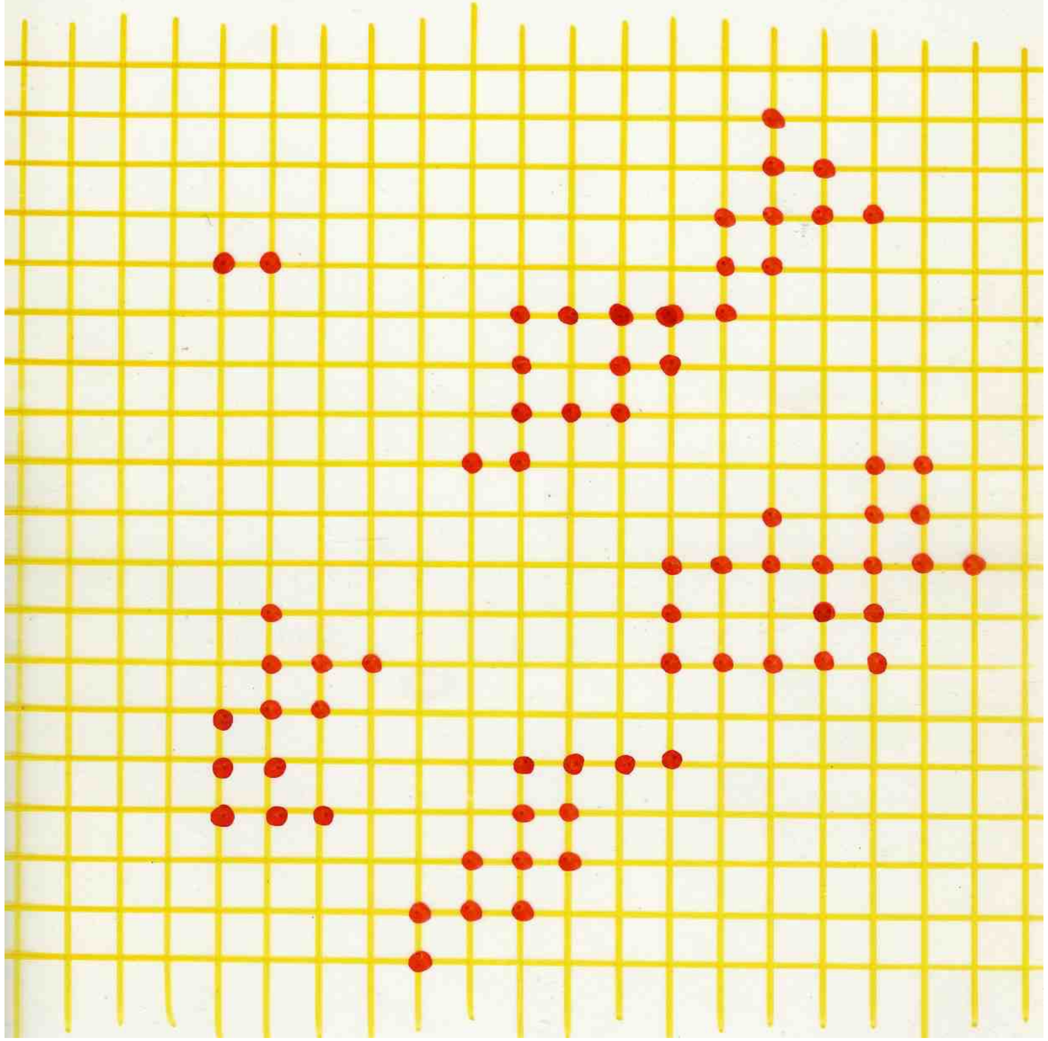
example 3

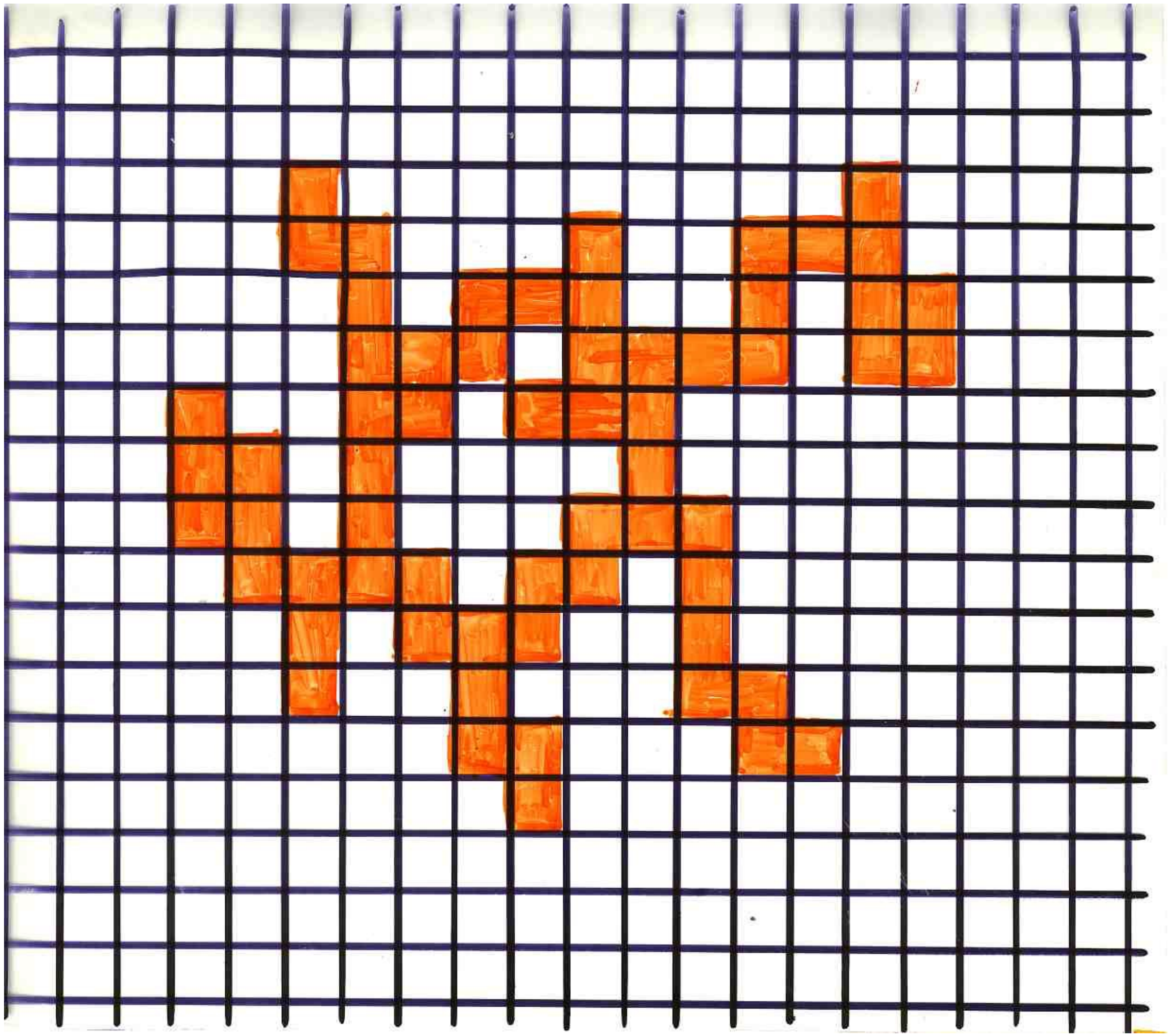
percolation

Percolation

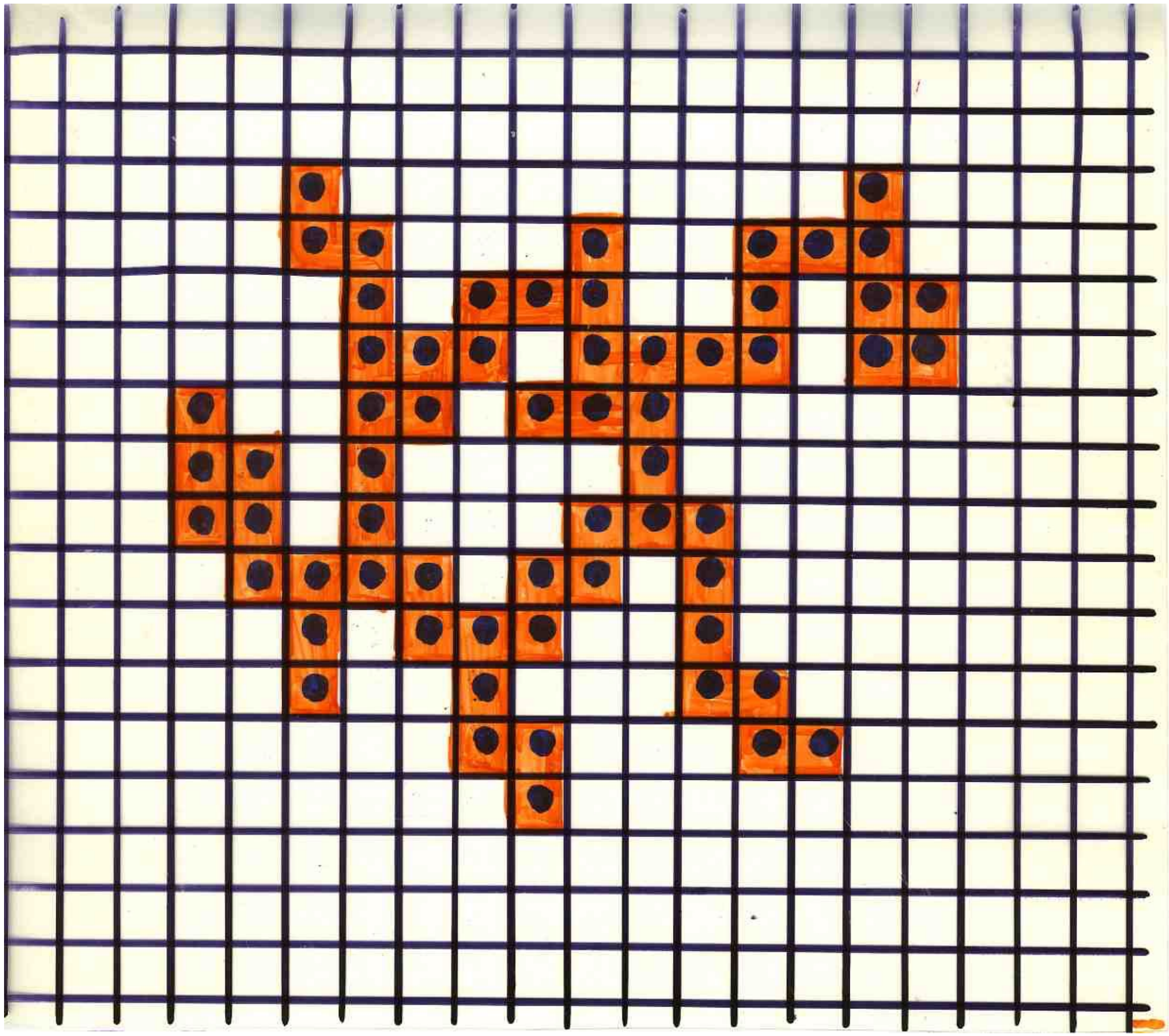


Percolation



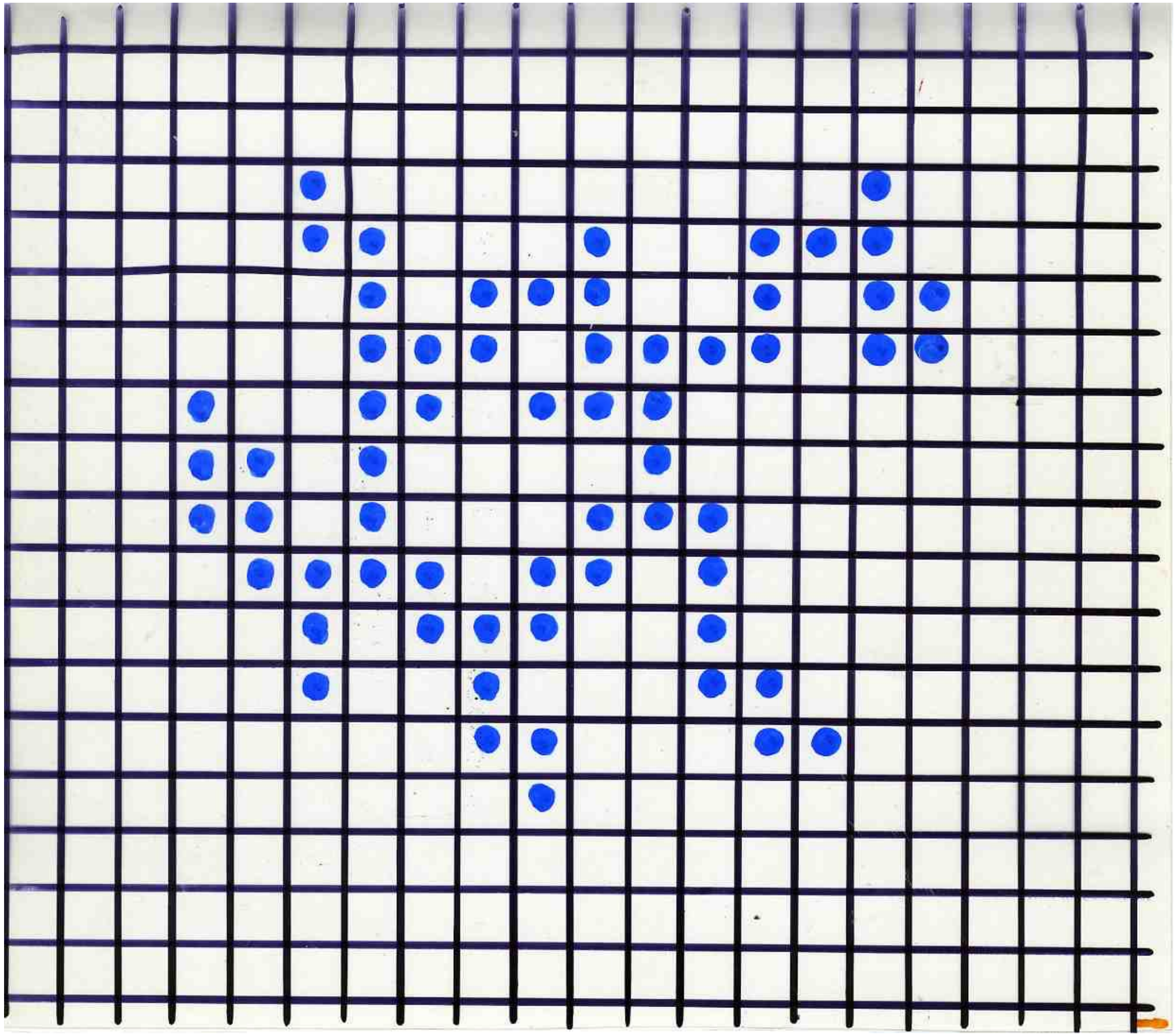


polyomino

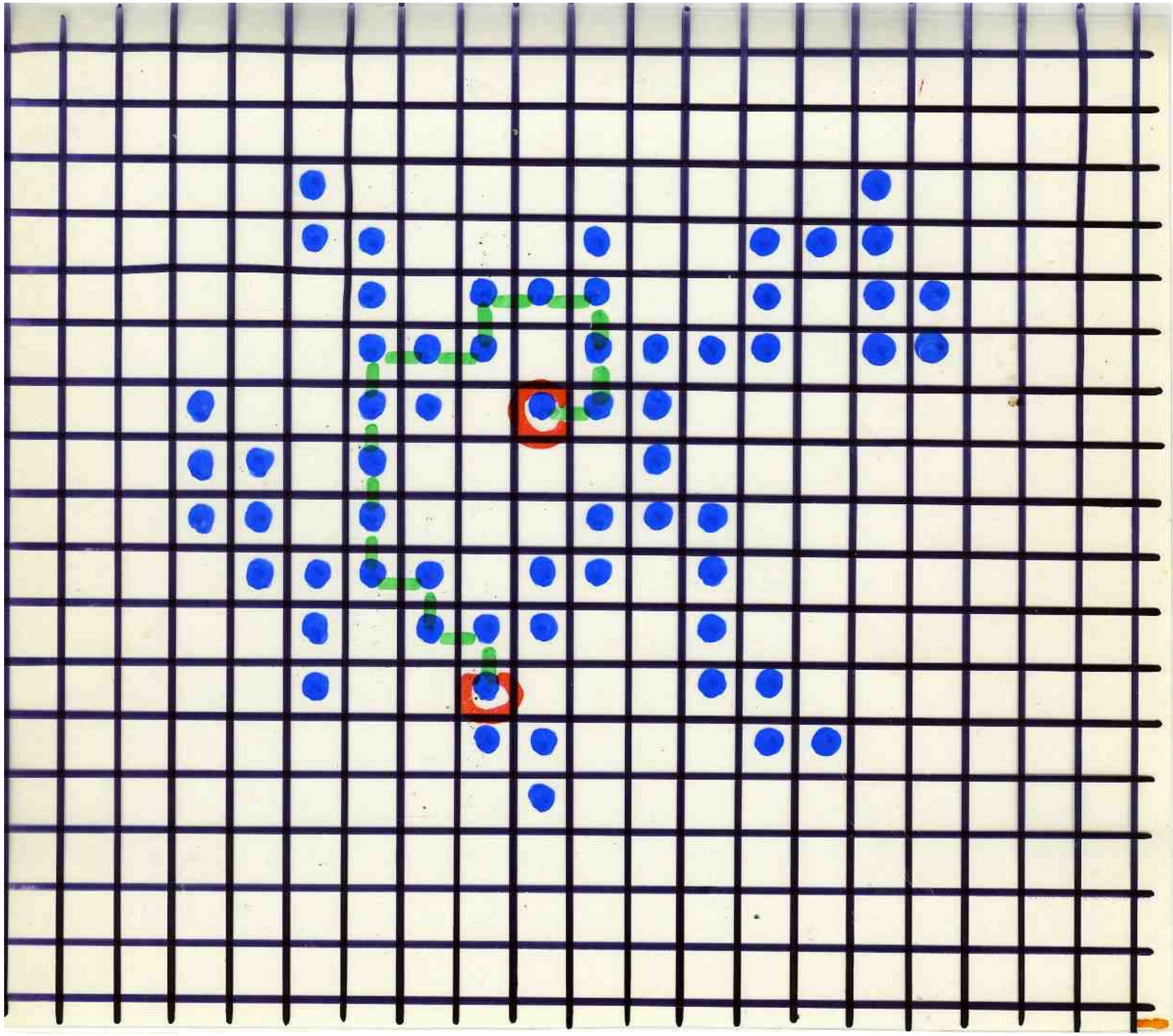


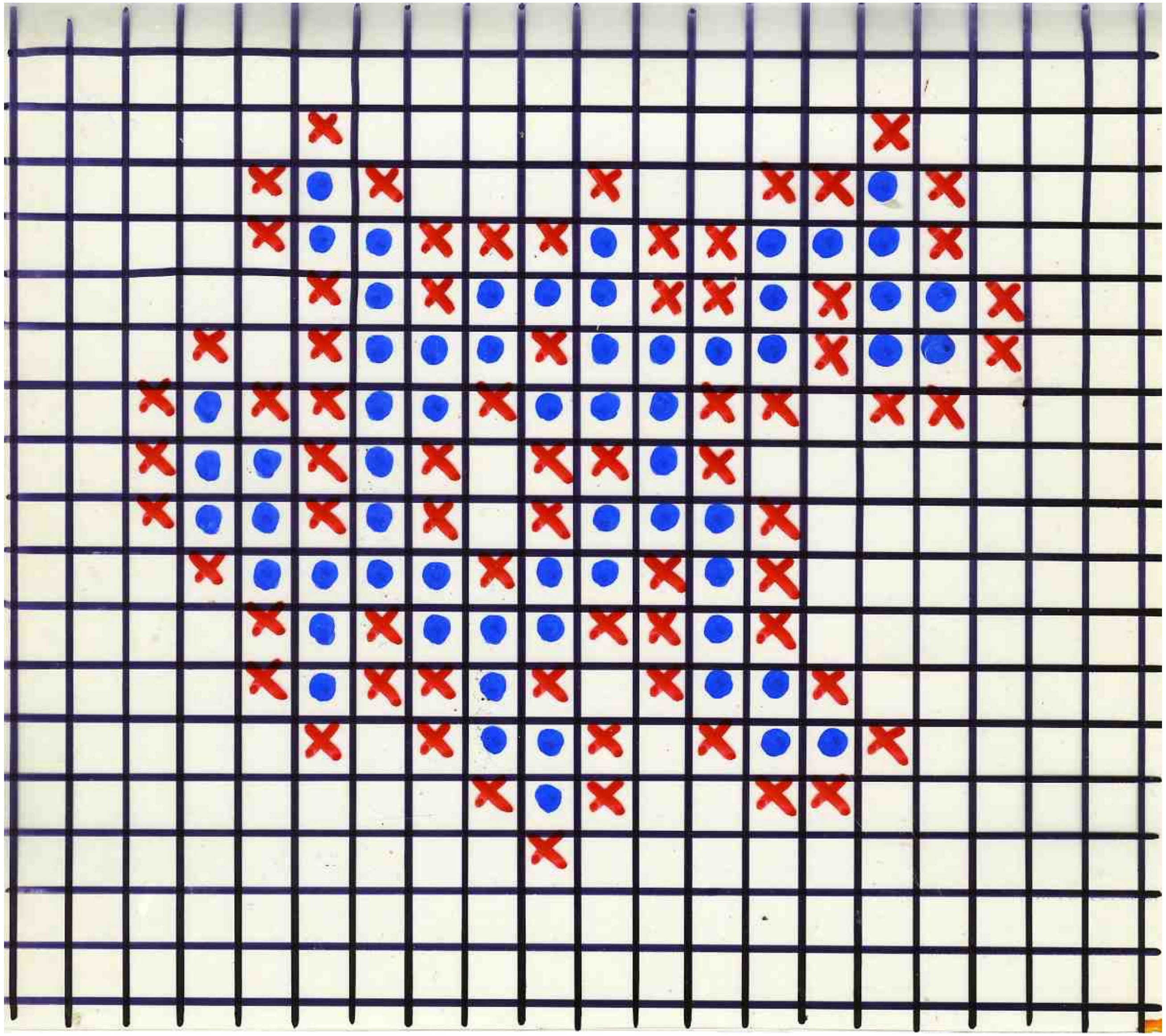
area

perimeter

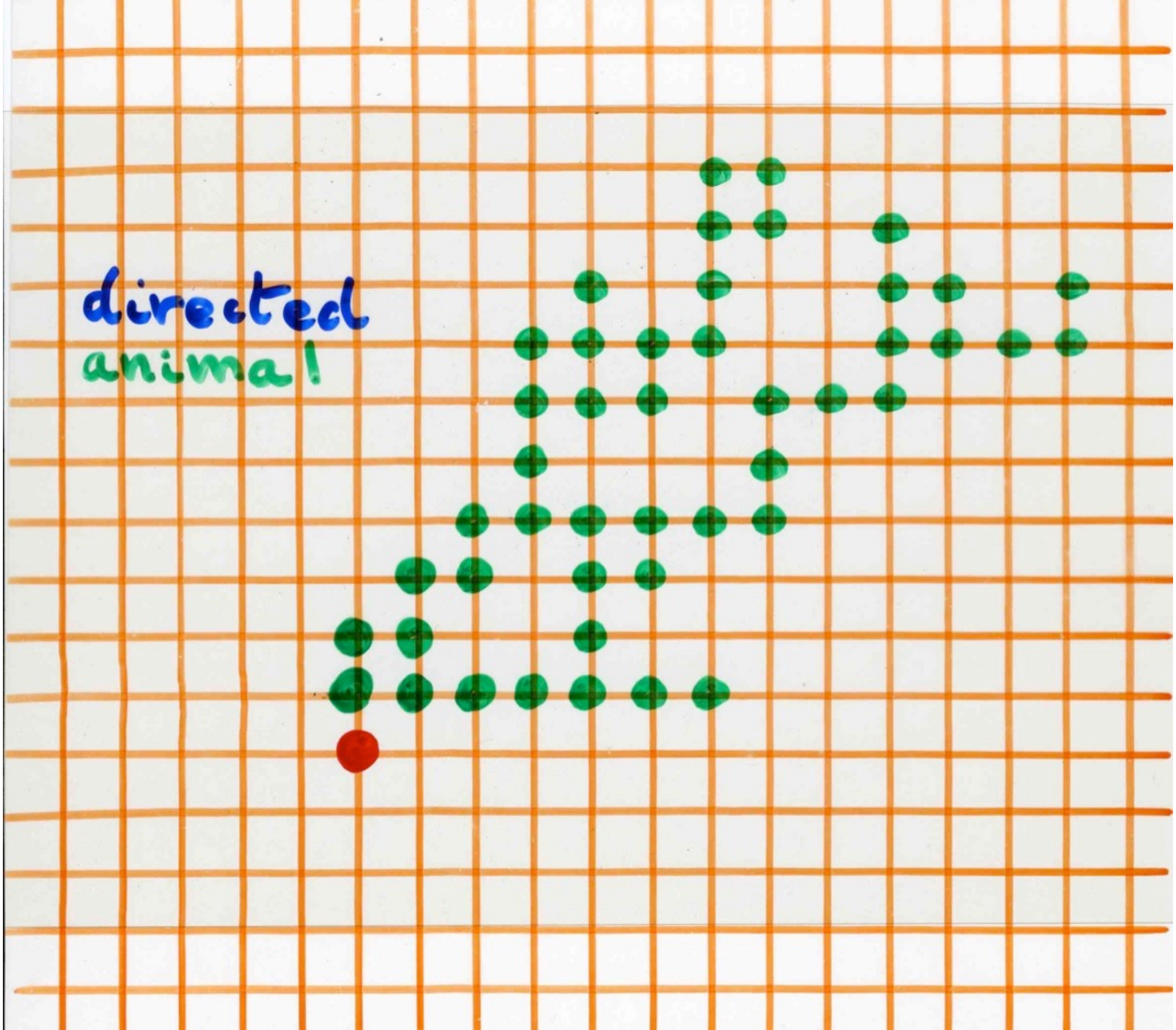


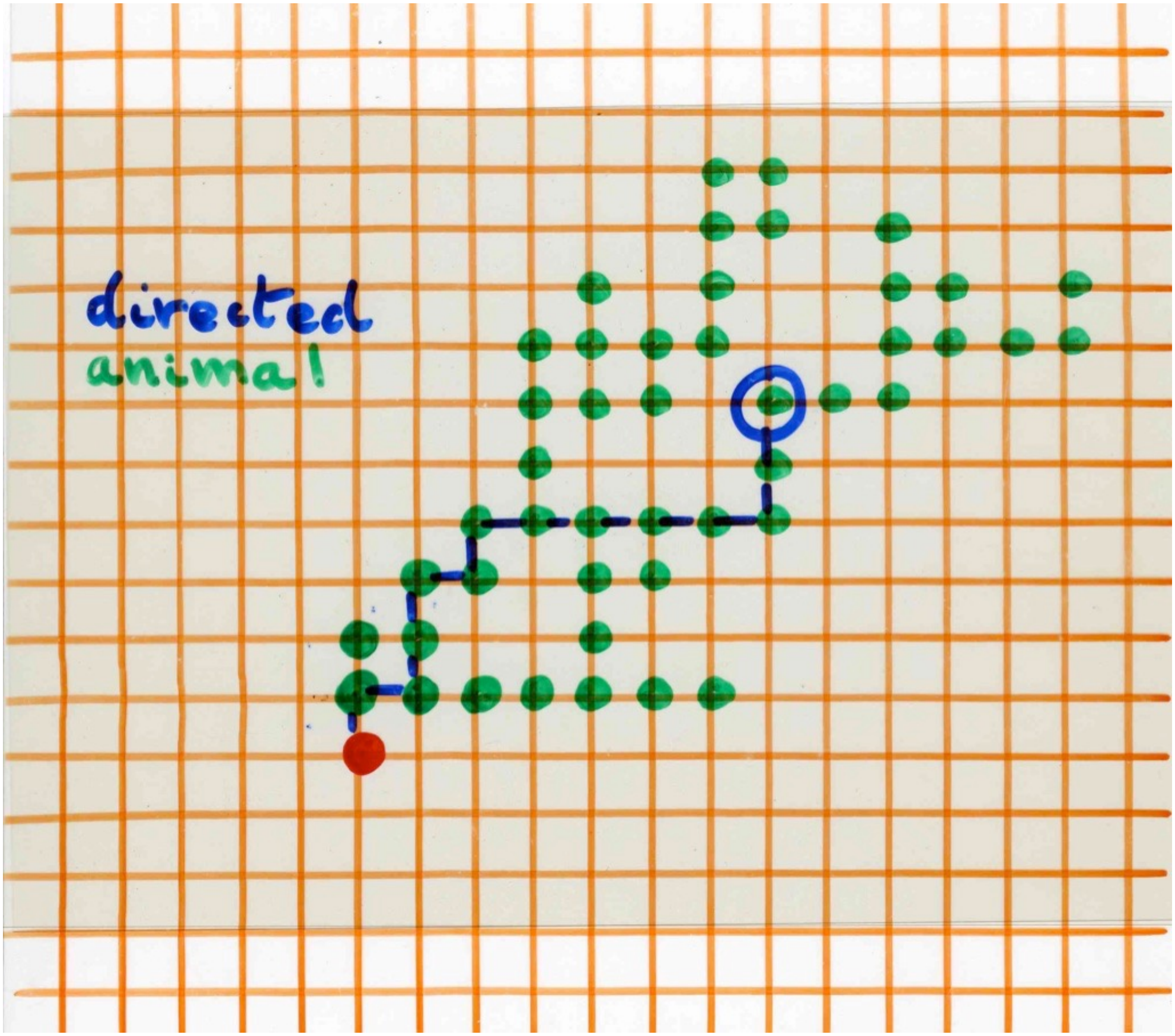
animal





The directed animal model

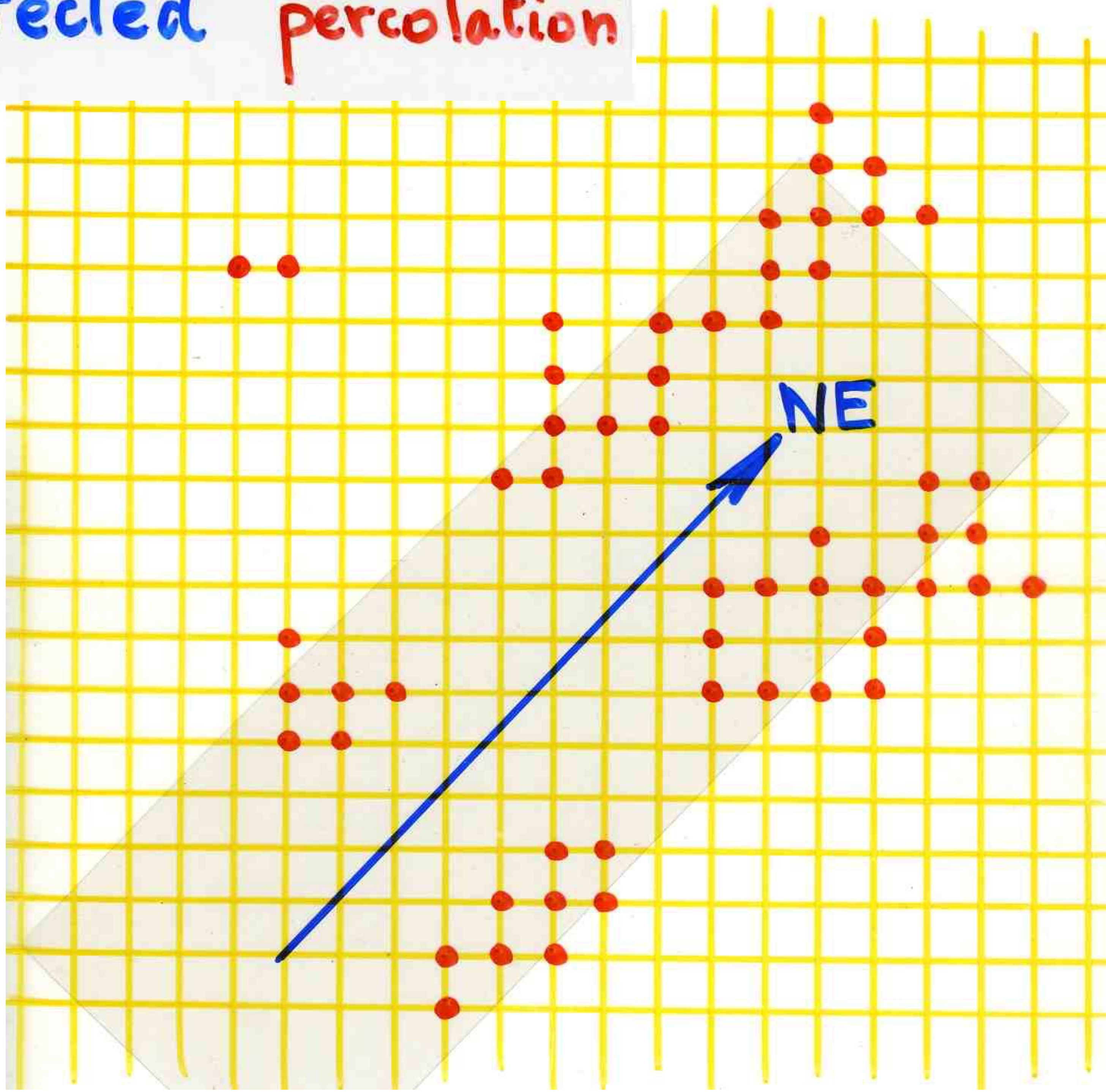

directed
animal

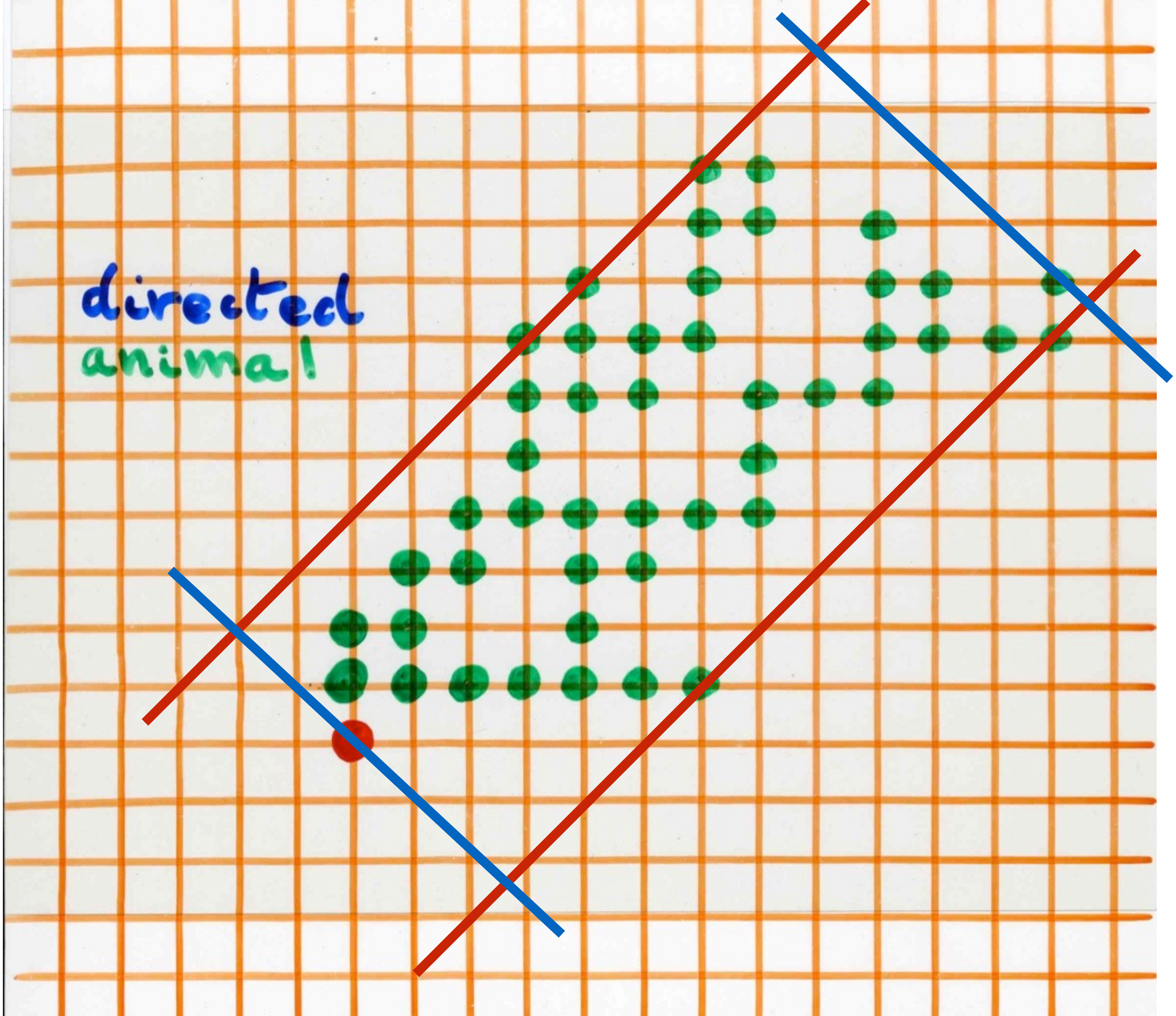

directed
animal

$a_n = \Big\{$ number of directed animals having n points

$$F(t) = \sum_{n \geq 1} a_n t^n$$

directed percolation




directed
animal

$$a_n \sim \mu^n \, n^{-\theta}$$

number of directed animals n points

$$\ell_n \sim n^{\nu_\perp}$$

average width

$$L_n \sim n^{\nu_\parallel}$$

average length

$$a_n \sim \mu^n \, n^{-\theta}$$

number of directed animals n points

$$\ell_n \sim n^{\nu_\perp}$$

average width

$$L_n \sim n^{\nu_\parallel}$$

average length

Critical exponents

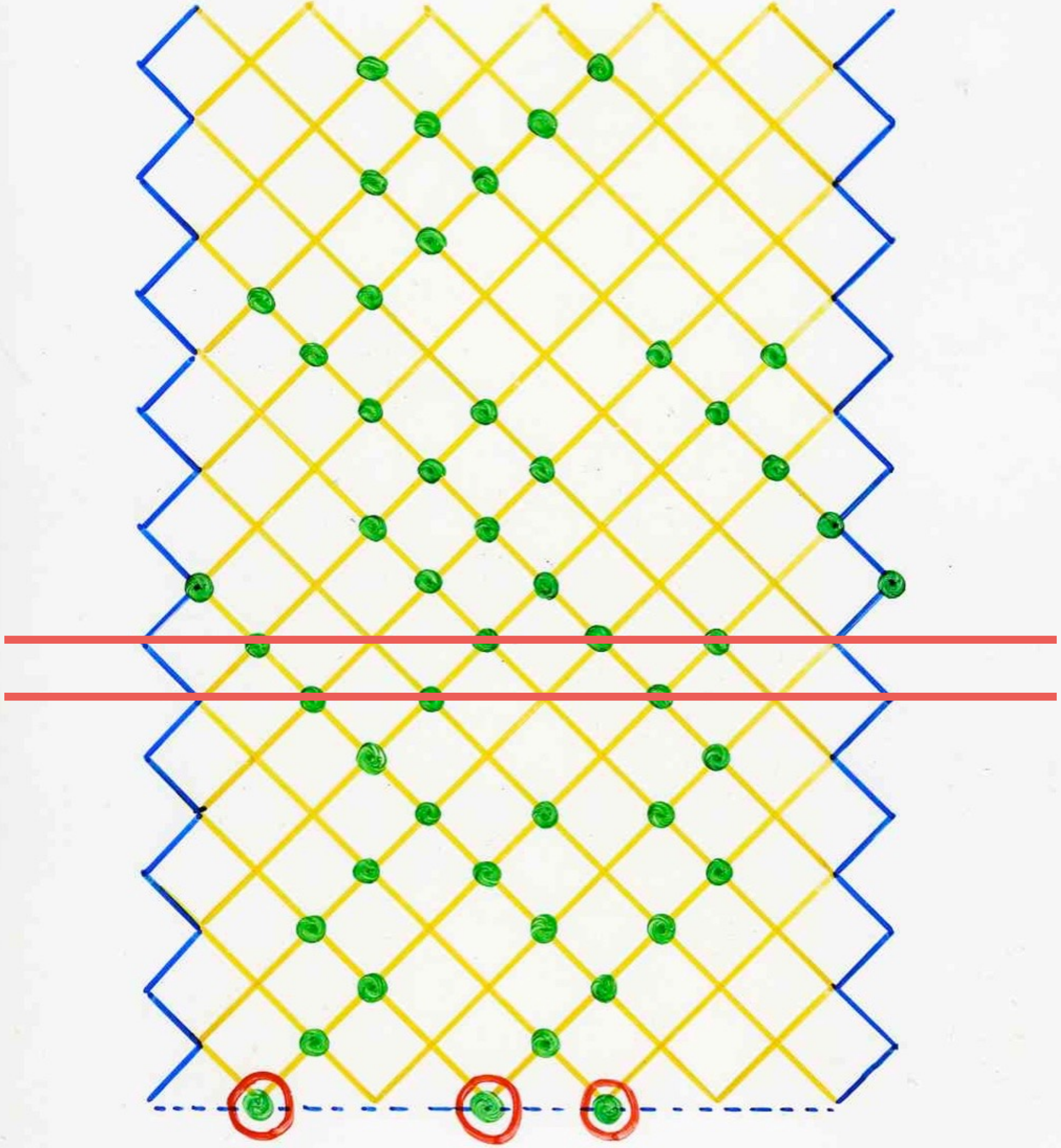
Nadal, Derrida, Vannimenus (1982)

B. Derrida

J. Vannimenus

J.P. Nadal

(1982, 1983)



source points

directed animal
on a circular strip

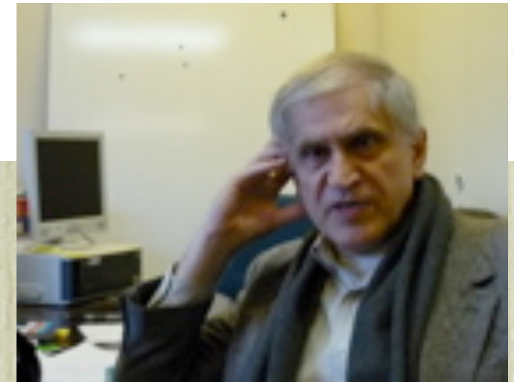
$$\tilde{b}_n^{\leq k} = \frac{1}{k} \sum_{p=0}^{k-1} (-1)^p \sin \alpha_p \prod_{i=1}^{k-1} \left(\frac{\sin (i+\frac{1}{2}) \alpha_p}{\sin \frac{\alpha_p}{2}} \right)^{N_i} (1 + 2\cos \alpha_p)^{n-1}$$

animals

circular strip

width k

$$\alpha_p = \frac{2p+1}{2k} \pi$$



J. Vannimenus

J.P. Nadal

(1982, 1983)

B. Derrida

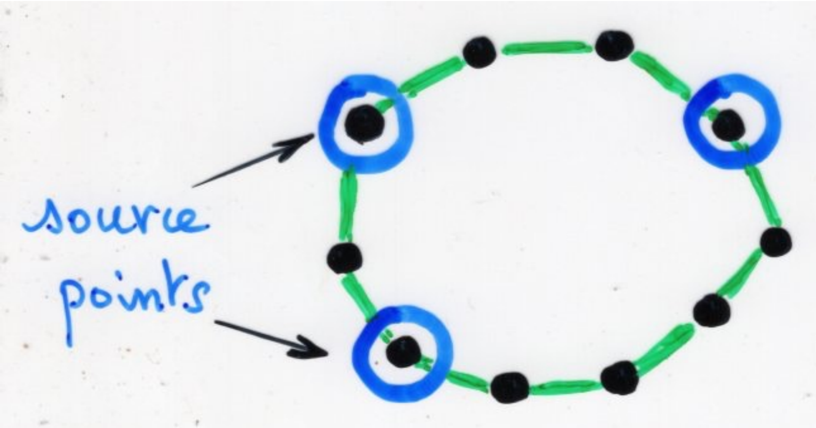
Nadal, Derrida, Vannimenus (1982)

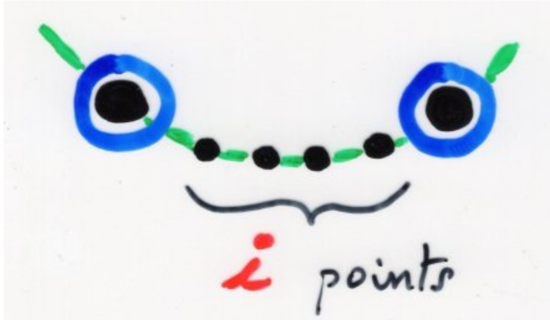
$$\tilde{b}_n^{\leq k} = \frac{1}{k} \sum_{p=0}^{k-1} (-1)^p \sin\alpha_p \prod_{i=1}^{k-1} \left(\frac{\sin(i+\frac{1}{2})\alpha_p}{\sin\frac{\alpha_p}{2}} \right)^{N_i} (1+2\cos\alpha_p)^{n-1}$$

animals
circular strip
width k

$$\alpha_p = \frac{2p+1}{2k}\pi$$

N_i = number of i-holes





Nadal, Derrida, Vannimenus (1982)

$a_n^k \sim c(\mu_k)^n$

$\mu_k = 1 + 2 \cos \pi/2k$

$a_n \sim \mu^n n^{-\theta}$

$\mu = 3 \quad \theta = 1/2$

$\nu_\perp = 1/2$

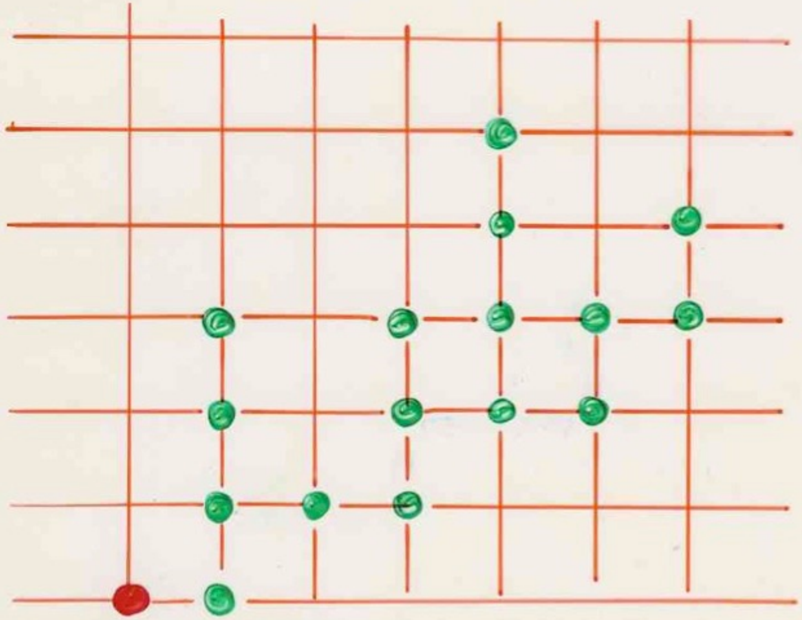
$\nu_\parallel = \cancel{9/11}$?

Hakim, Nadal (1982)

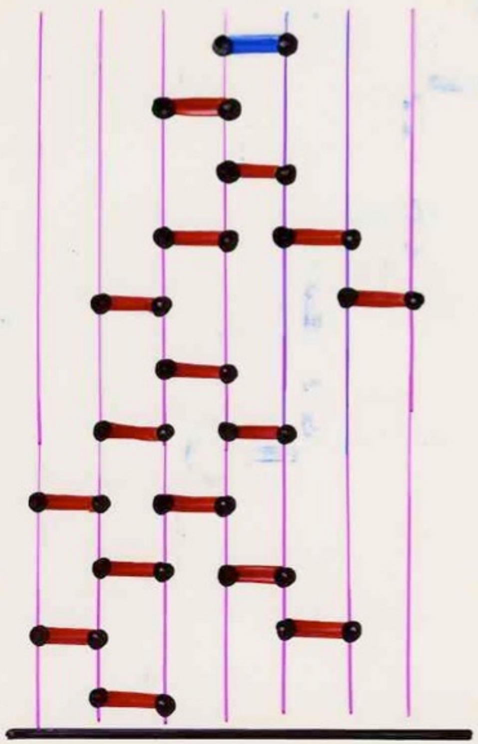
D. Dhar (1982)

directed animals

and heaps of dimers

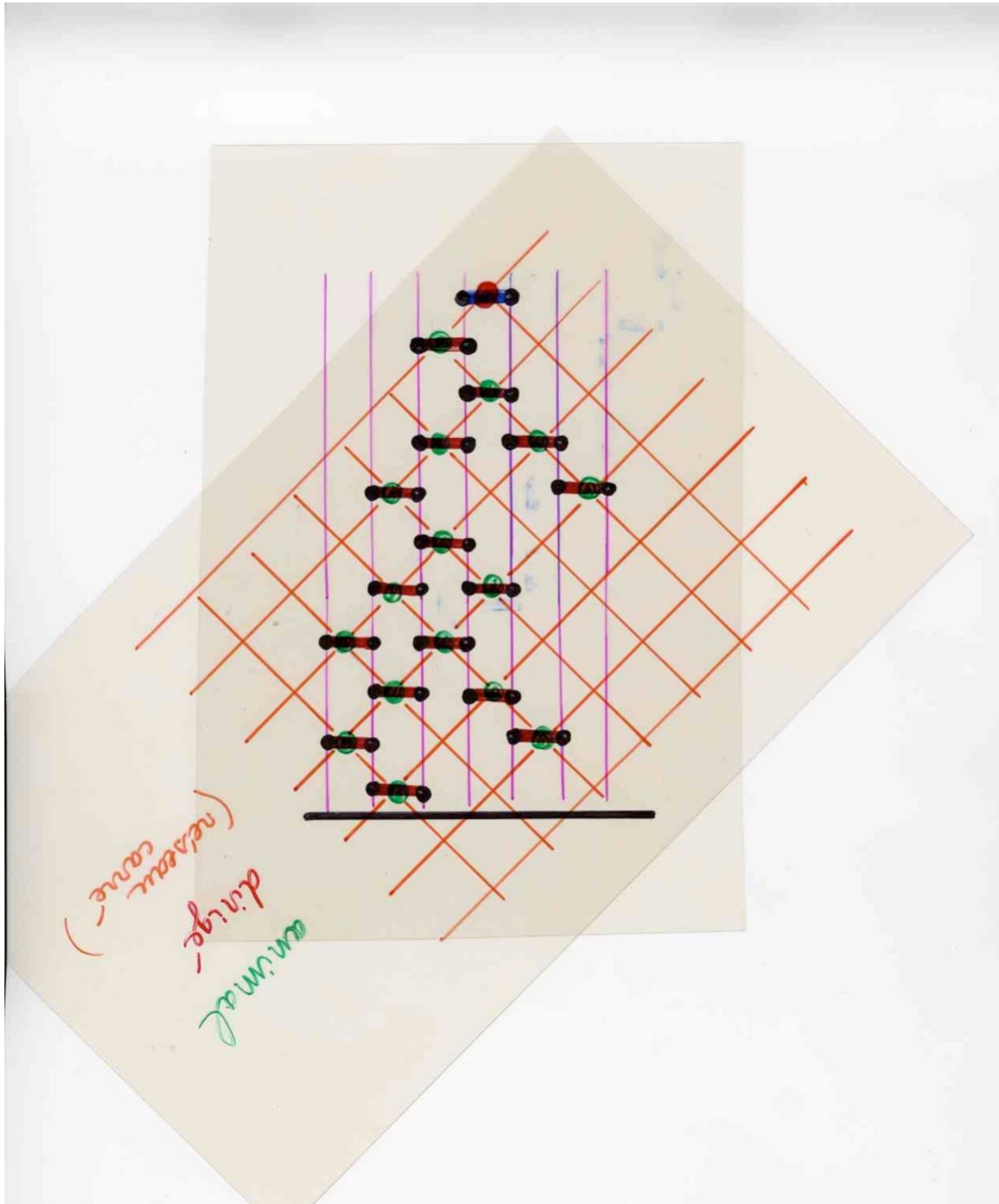


directed
animal
(square
lattice)

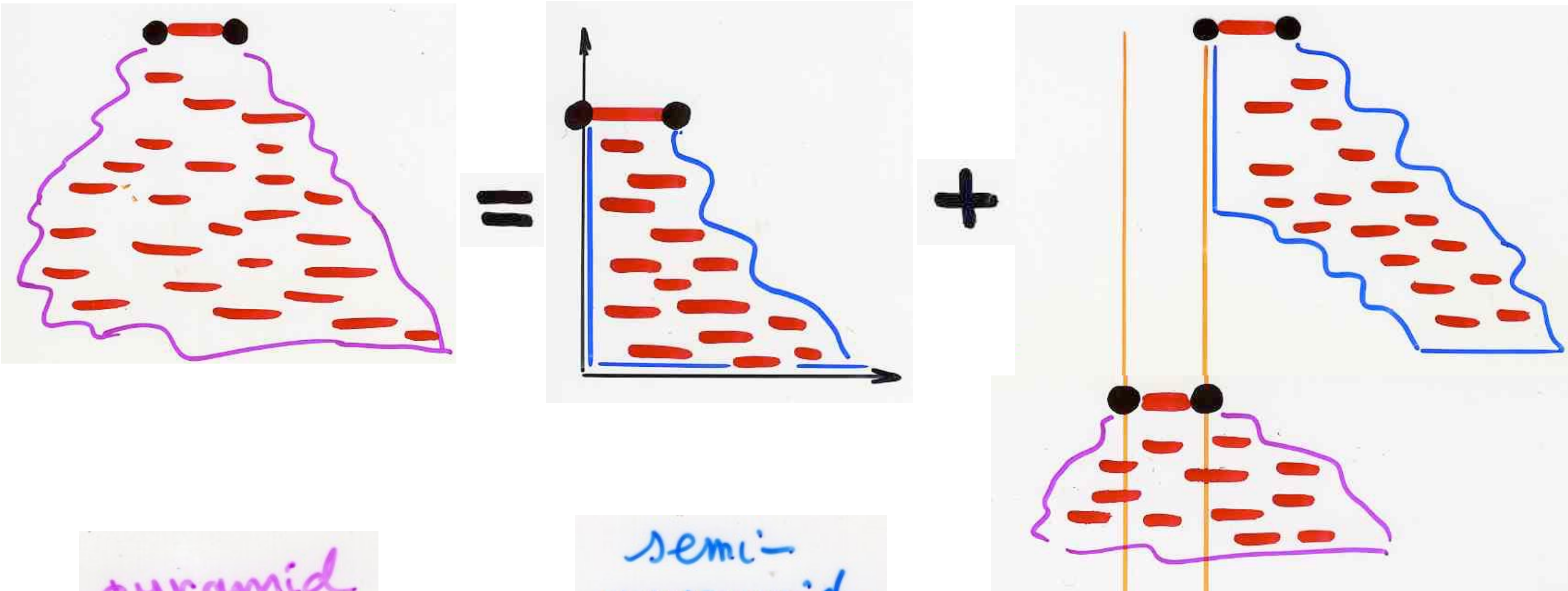


strict
pyramids

bijection



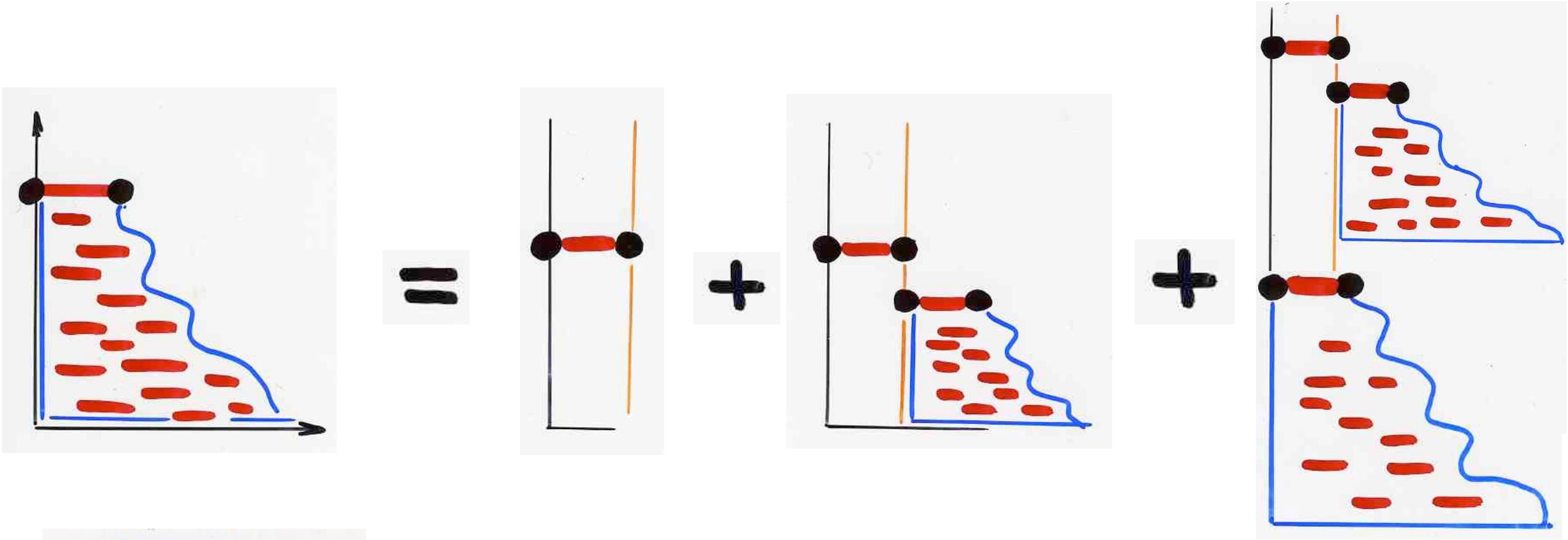
strict
pyramids



pyramid

semi-pyramid

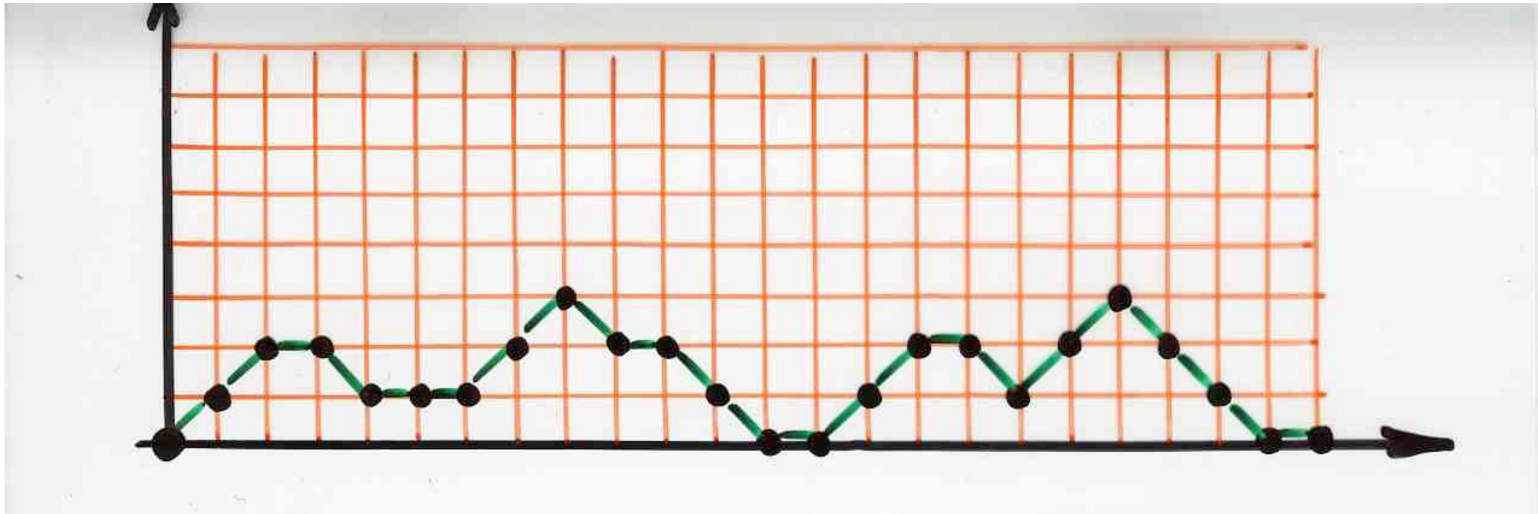
$$P = H + PH$$



semi-
pyramid

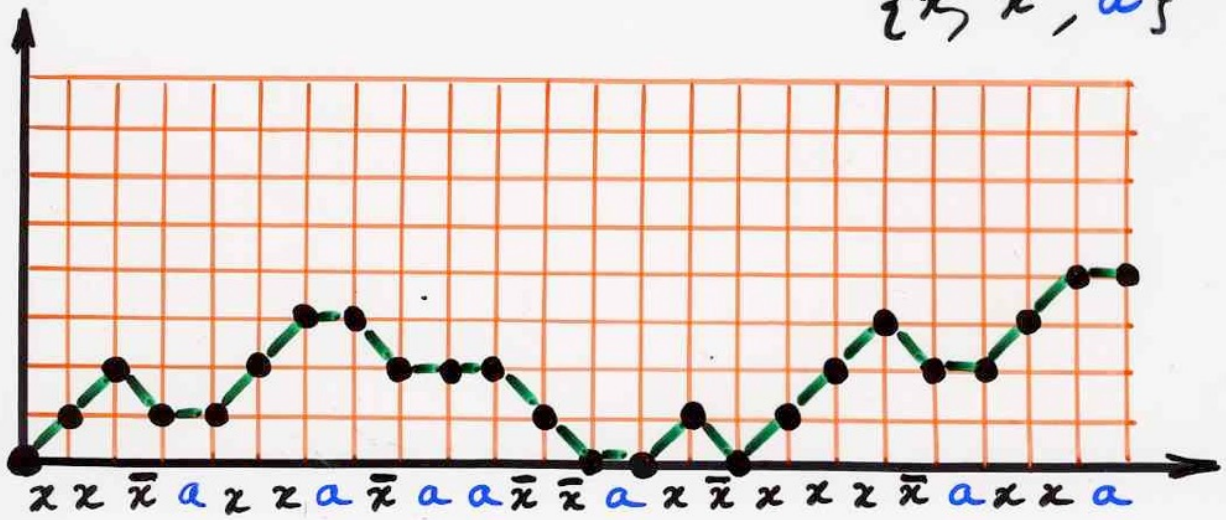
$$H = z + zH + zH^2$$

Motzkin paths



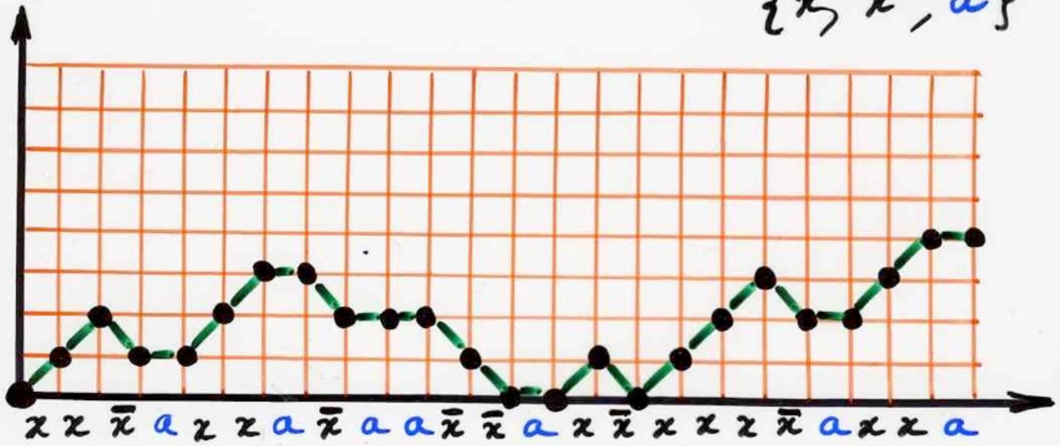
prefix (left factor) of a Motzkin path

(word) $\{x, \bar{x}, a\}$



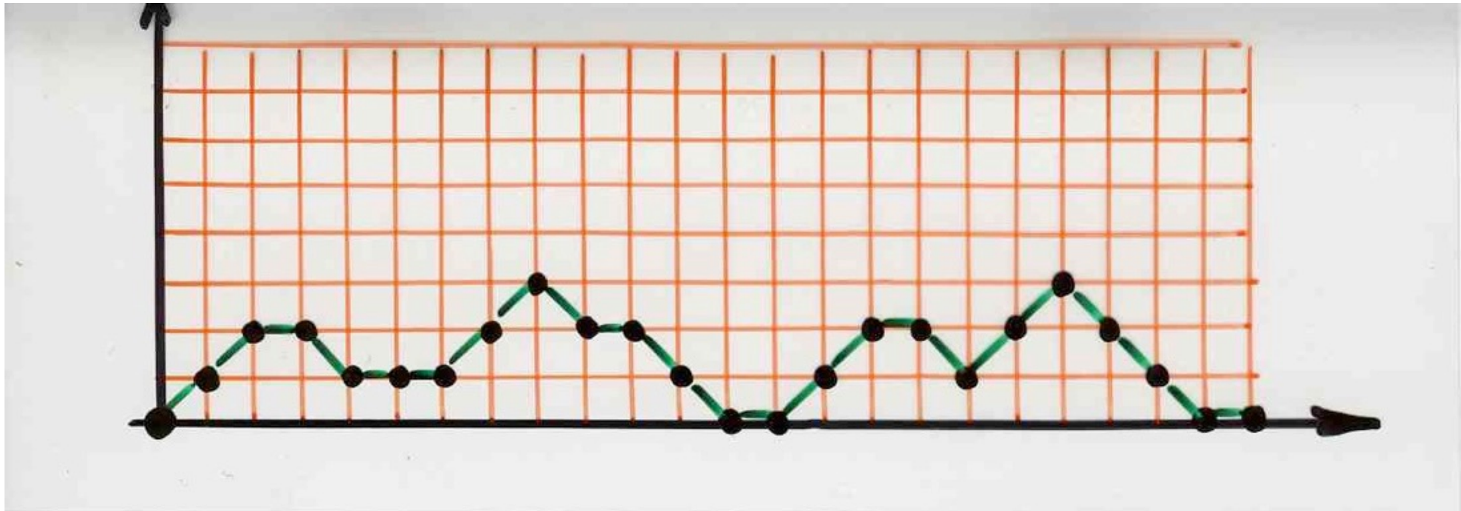
prefix (left factor) of a Motzkin path (word)

$\{x, \bar{x}, a\}$



- prefix Motzkin path $=$ $\begin{cases} \bullet \text{ Motzkin path} \\ \bullet \text{ (Motzkin path)} \times \text{( )} \times \text{(prefix Motzkin path)} \end{cases}$

$$p = m + t\,p\,m$$



- Motzkin path =
$$\begin{cases} \bullet \quad \emptyset \\ \bullet \quad (\bullet\!-\!\bullet) \times (\text{Motzkin path}) \\ \bullet \quad (\nearrow) \times (\text{Motzkin path}) \times (\searrow) \times (\text{Motzkin path}) \end{cases}$$

$$m = 1 + t\,m + t^2 m^2$$

$$P = H + PH$$

$$H = z + zH + zH^2$$

$$P = t_P$$
$$H = t_m$$

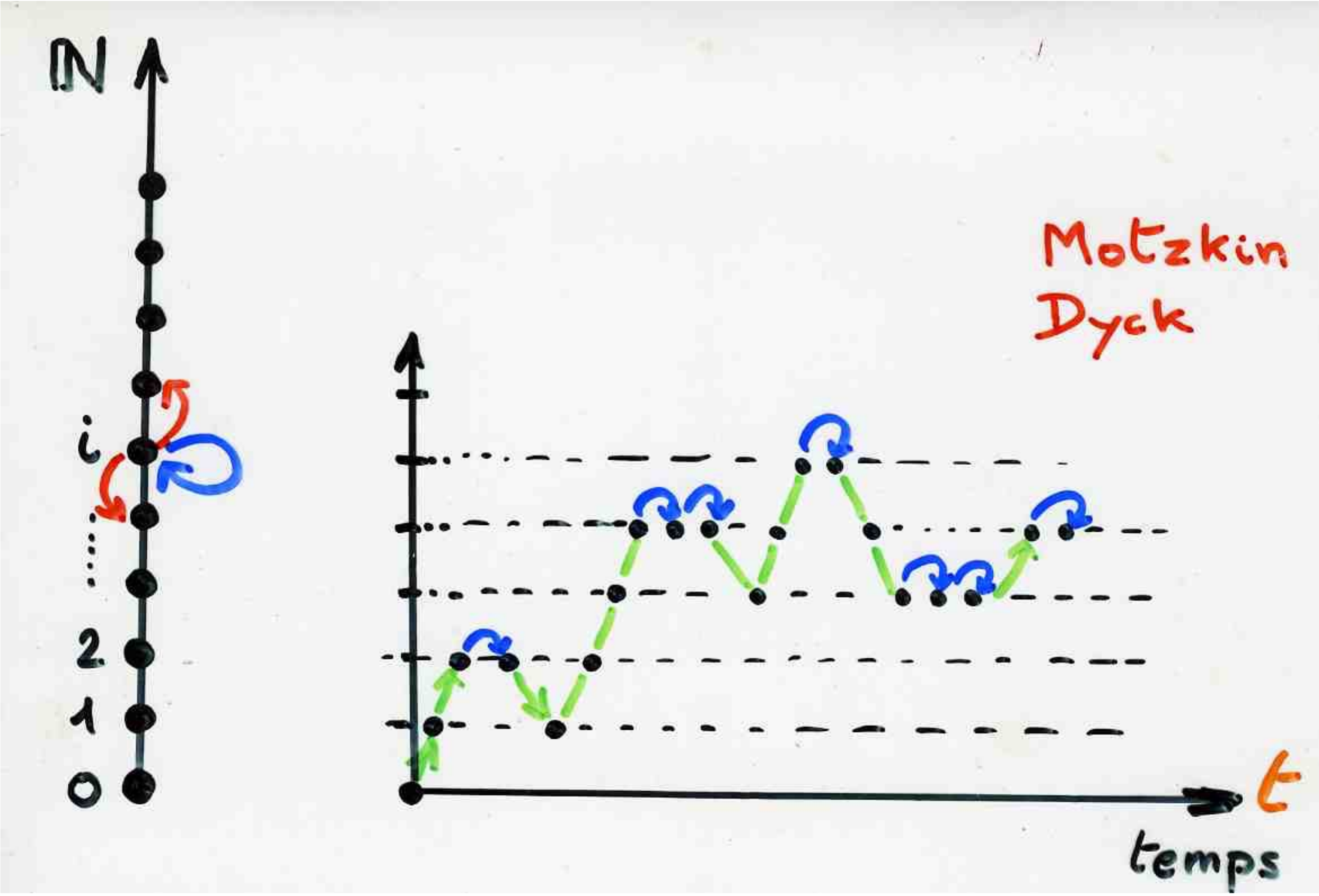
number of directed animals n points = number of prefix of Motzkin paths length $(n-1)$

(Brute force) bijection

2d animals → 1d paths

D. Gouyou-Beauchamps

X. V. (1984)



$$\sum_{n \geq 1} a_n t^n = \frac{1}{2}\left[\left(\frac{1+t}{1-3t}\right)^{1/2} - 1\right]$$

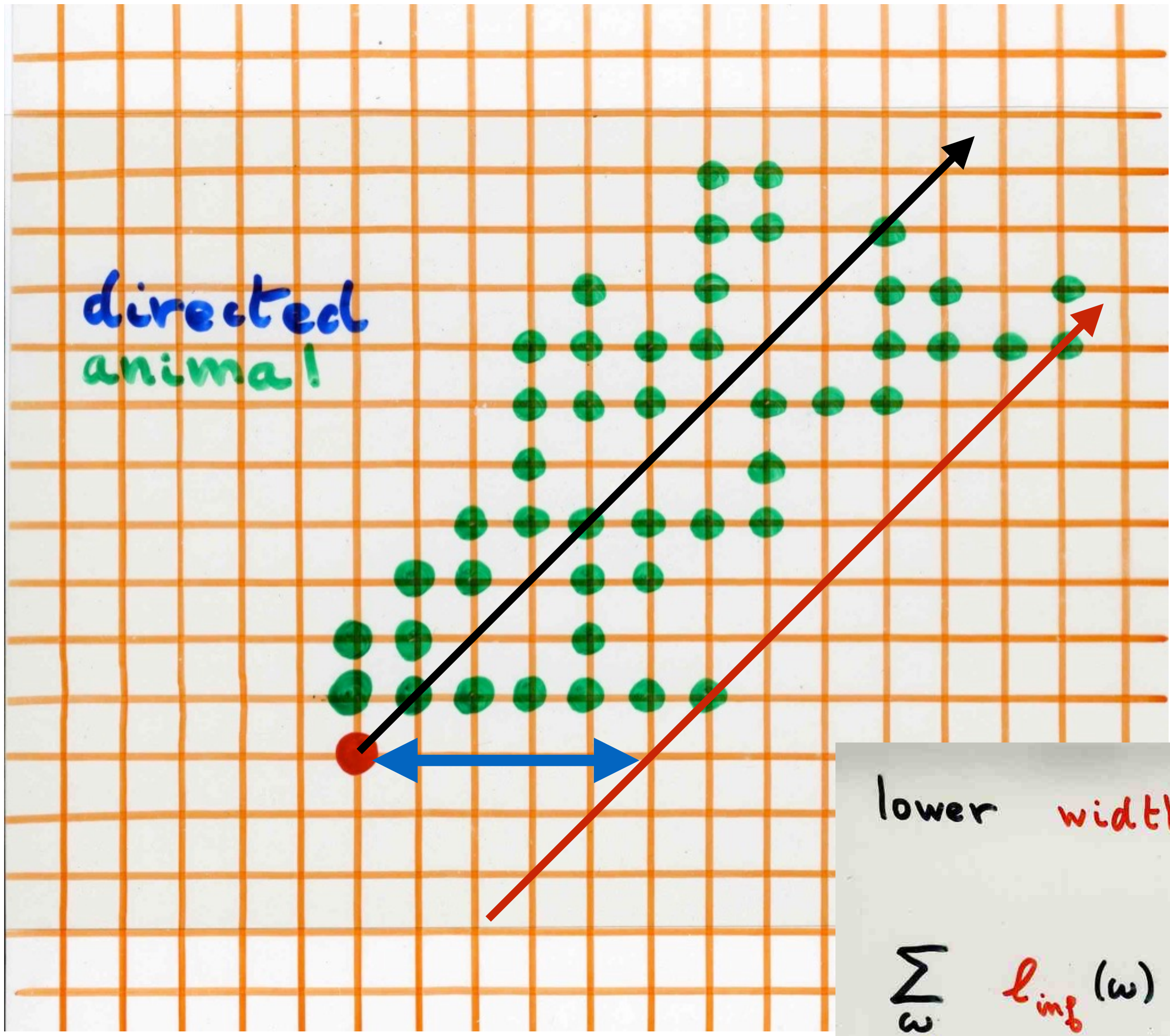
$$a_{n+1} = \sum_{0 \leq i \leq n} \binom{n}{i} \binom{i}{\lfloor i/2 \rfloor}$$

lower width → level of the final point of the path

$$\sum_{\substack{\omega \\ \text{path} \\ |\omega| = n}} \ell_{\inf}(\omega) = 3^n$$

$$\ell_{n+1} = \frac{2 \cdot 3^n}{a_{n+1}} - 2$$ (Dhar conjecture) 1982

$\ell_n \sim n^{1/2}$ $\qquad \nu_\perp = \frac{1}{2}$

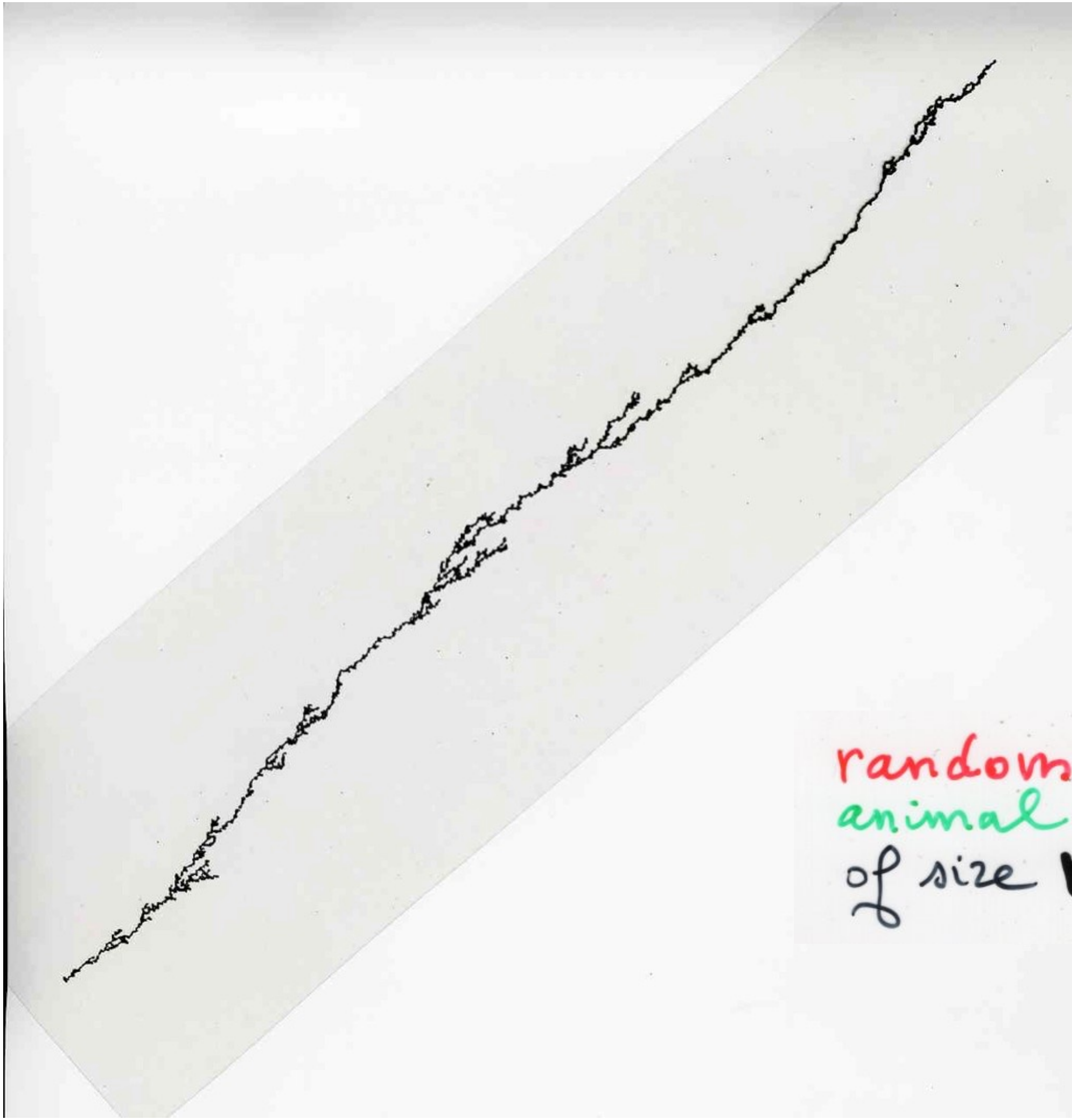


lower width → level of the final point of the path

$$\sum_{\substack{\omega \\ \text{path} \\ |\omega|=n}} \ell_{inf}(\omega) = 3^n$$

$$\ell_{n+1} = \frac{2.\,3^n}{a_{n+1}} - 2$$ (Dhar conjecture 1982)

$\ell_n \sim n^{1/2}$ $\qquad \nu_\perp = \frac{1}{2}$



random
animal
of size n

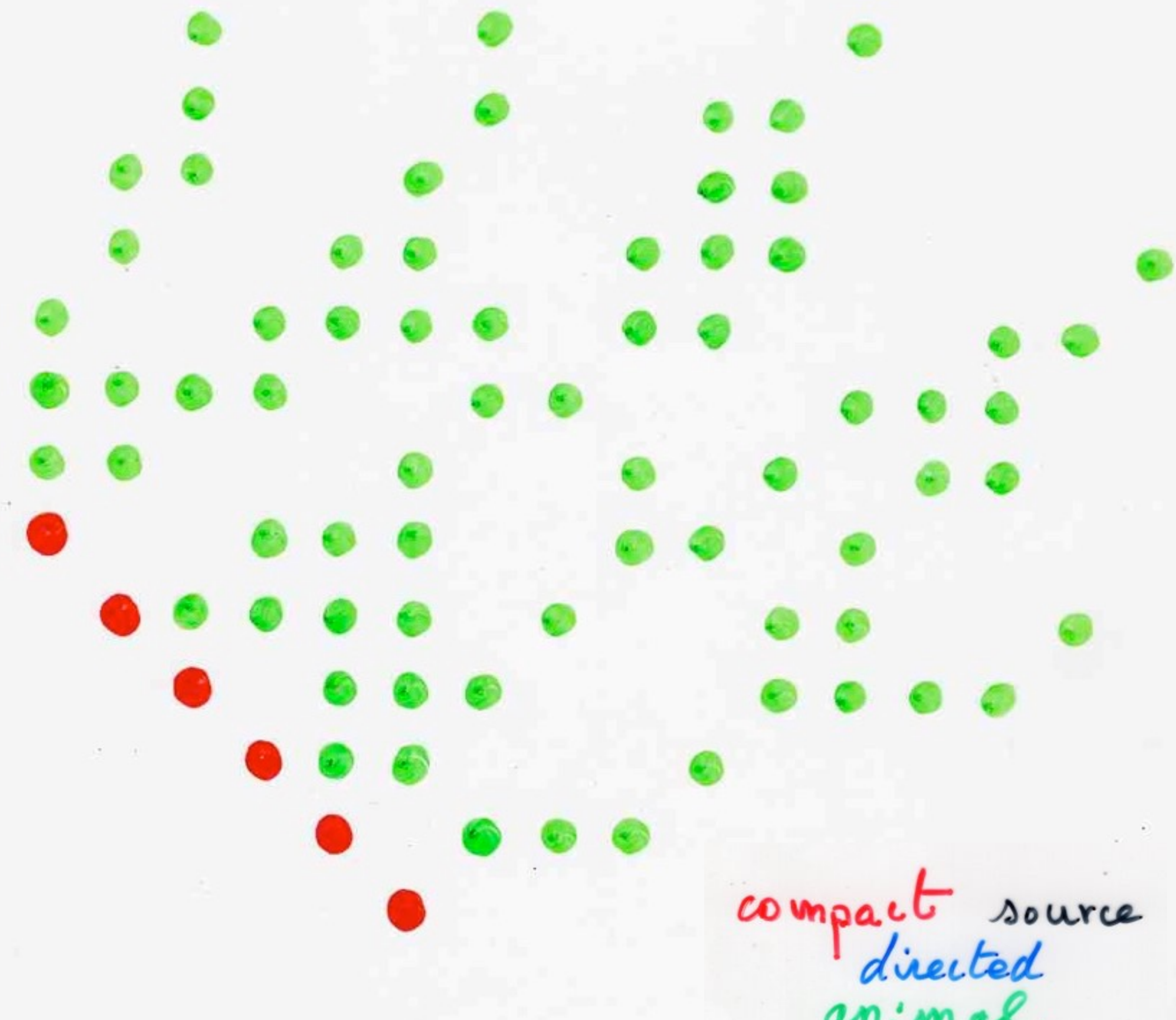
random
animal
of size n

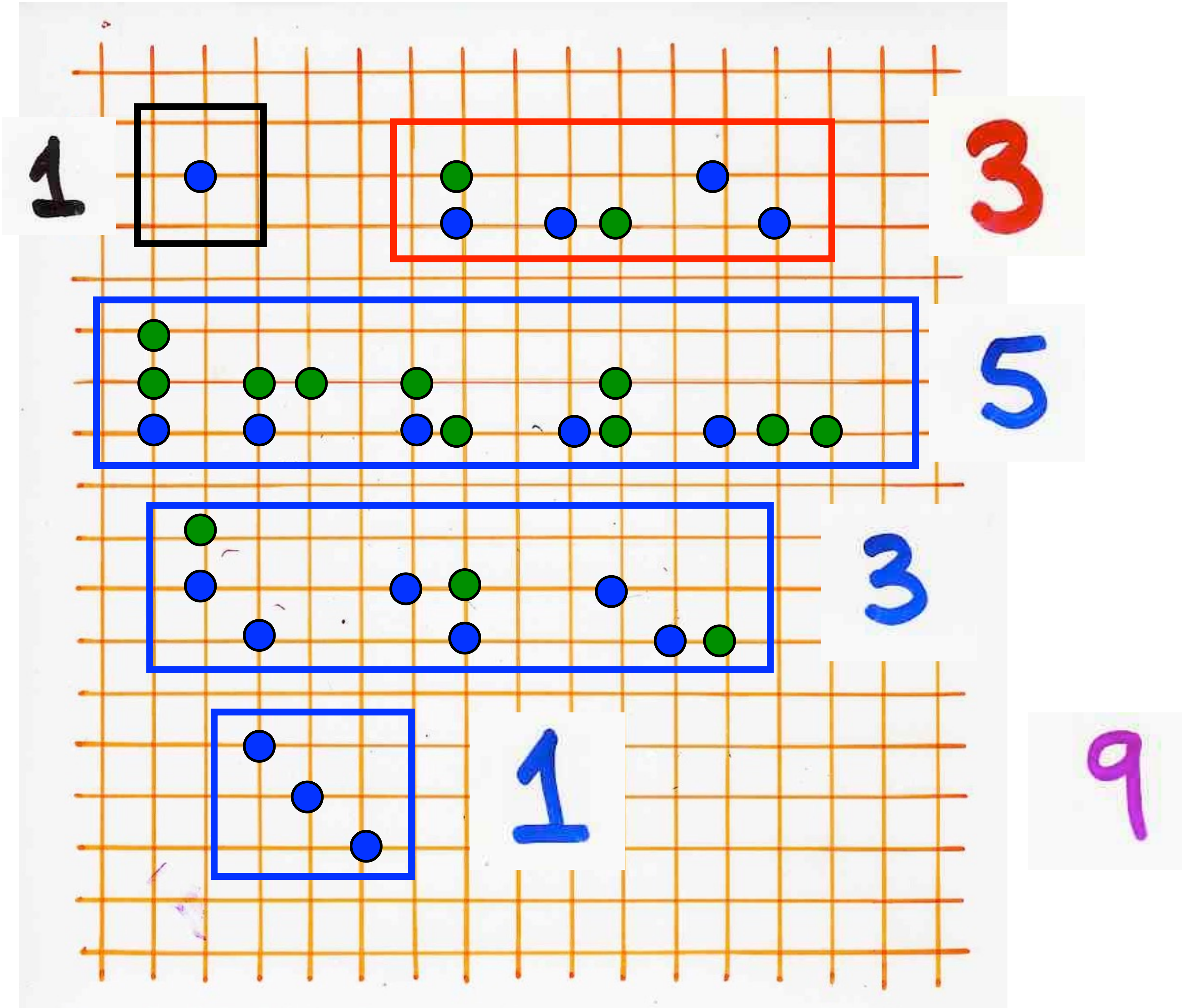
complements

exercise ?

compact source

directed animals

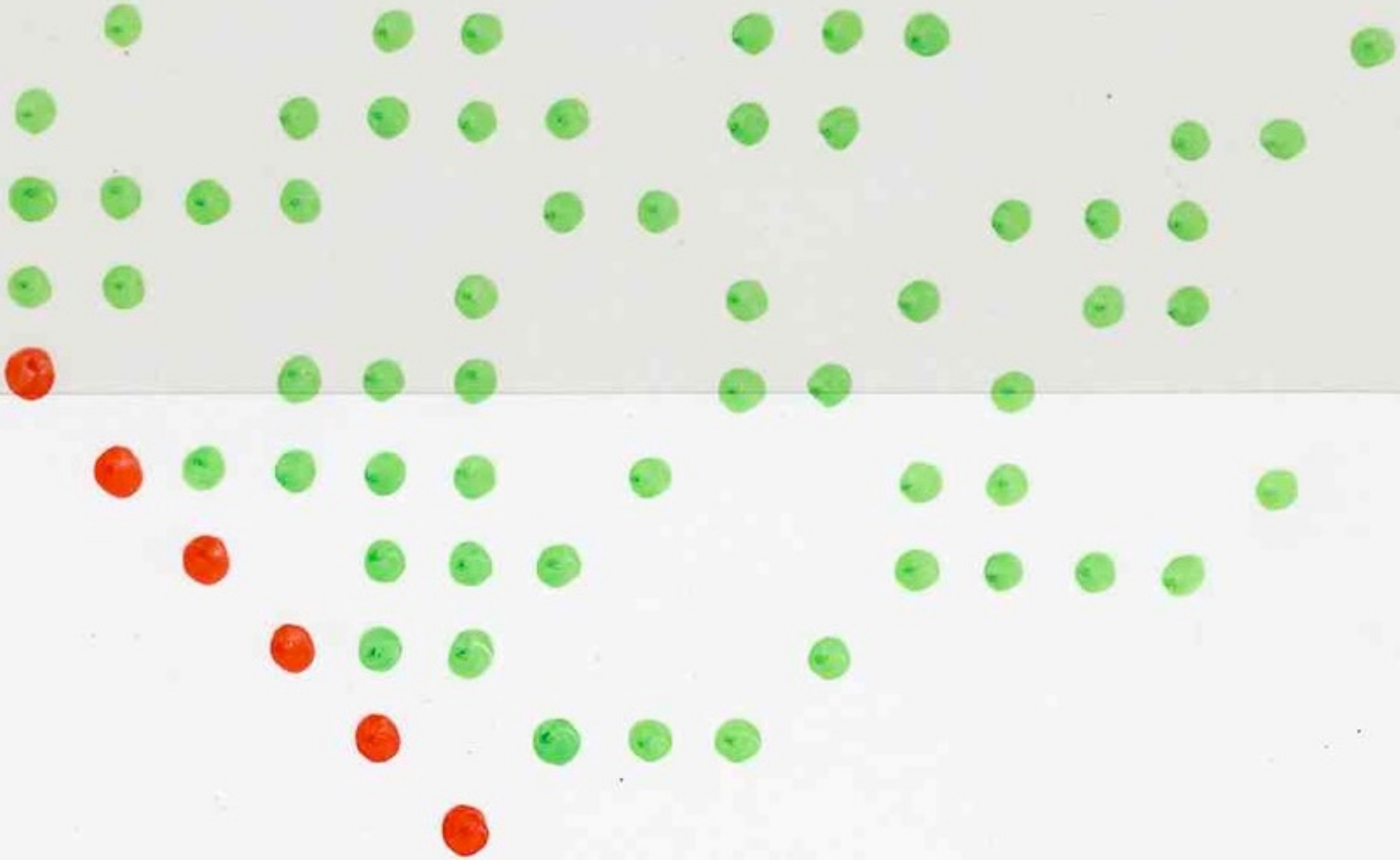

compact source
directed
animal


1
3
5
3
1
9

$1, 3, 9, 27, 81, \ldots$

$1, 3, 3^2, 3^3, 3^4, 3^5, 3^6,$!

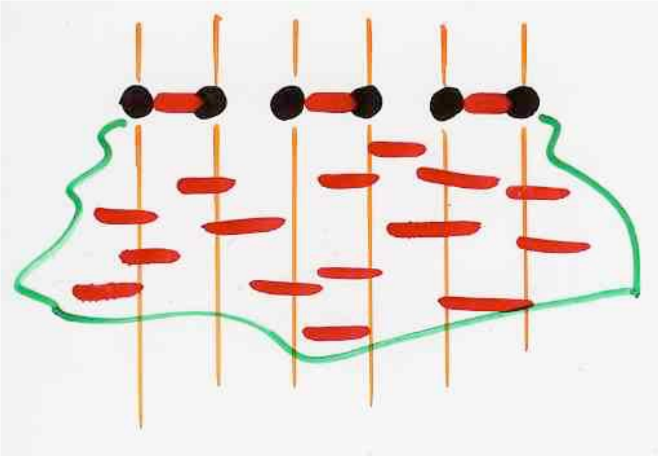
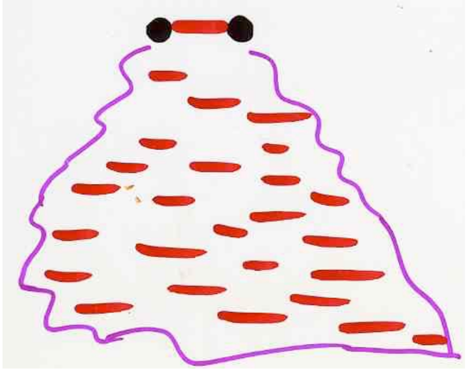
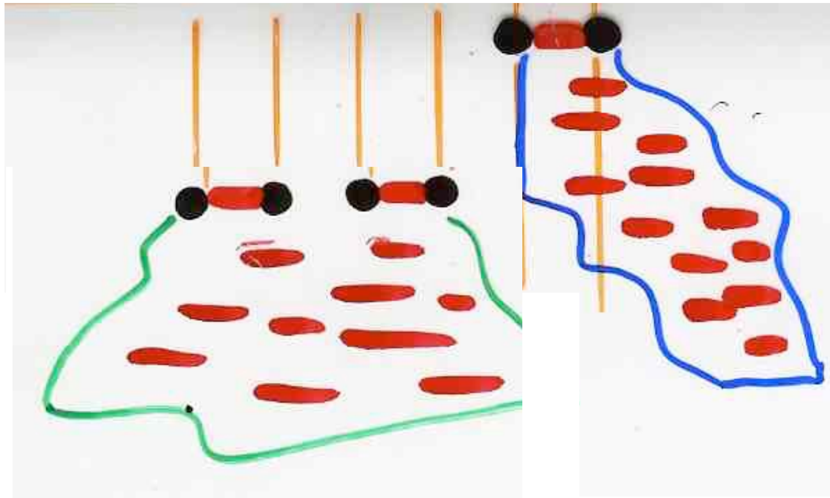
The number of directed animals size n+1, with compact source is



The number of directed animals
size n+1 , with compact source
is

$$3^n \; !$$

D. Gouyou-Beauchamps
X. V. (1984)

compact source
directed
animal

pyramid

semi-
pyramid

$$X = P + XH$$

$$H = z + zH + zH^2$$

$$P = H + PH$$

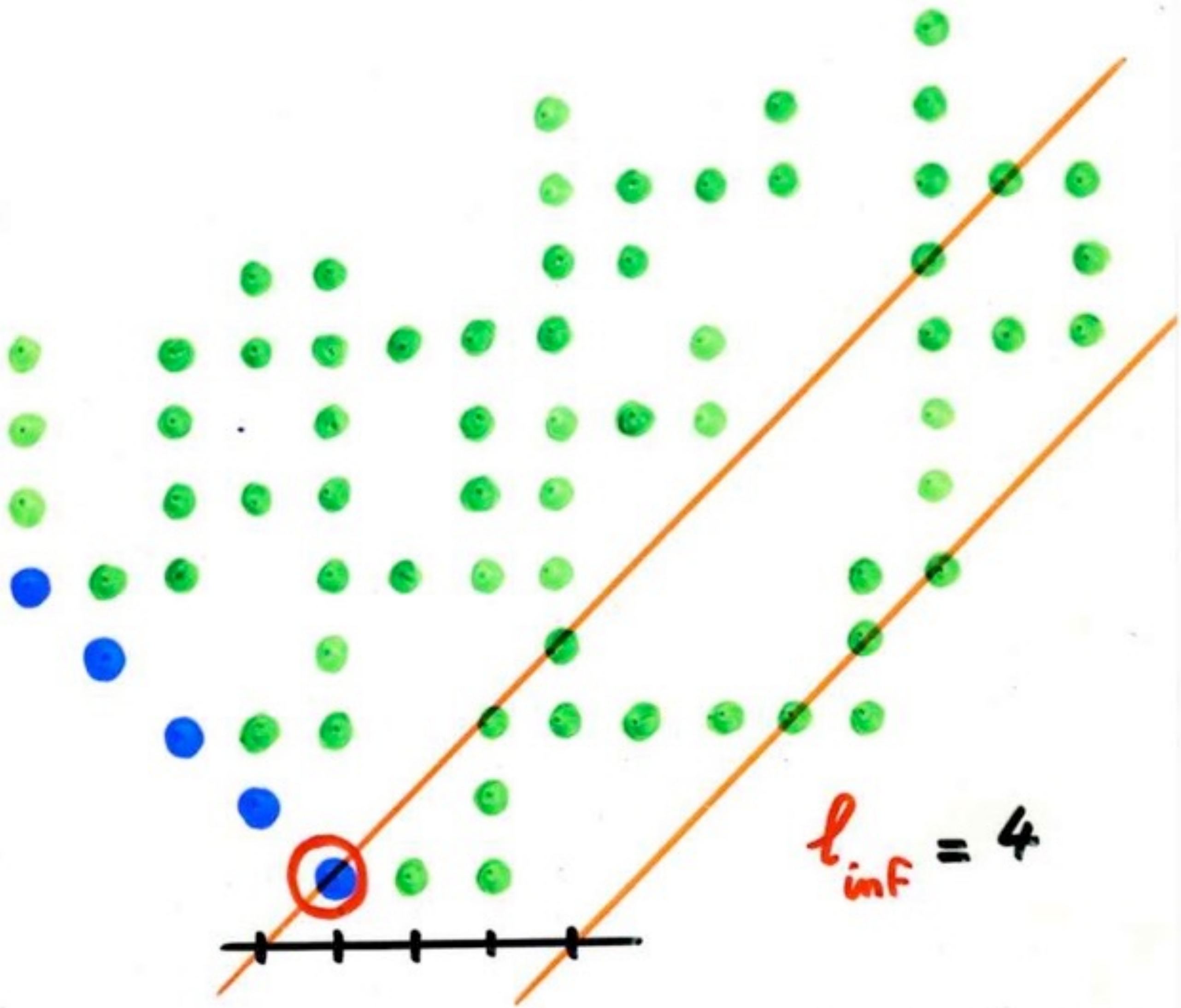
$$X = P + XH$$

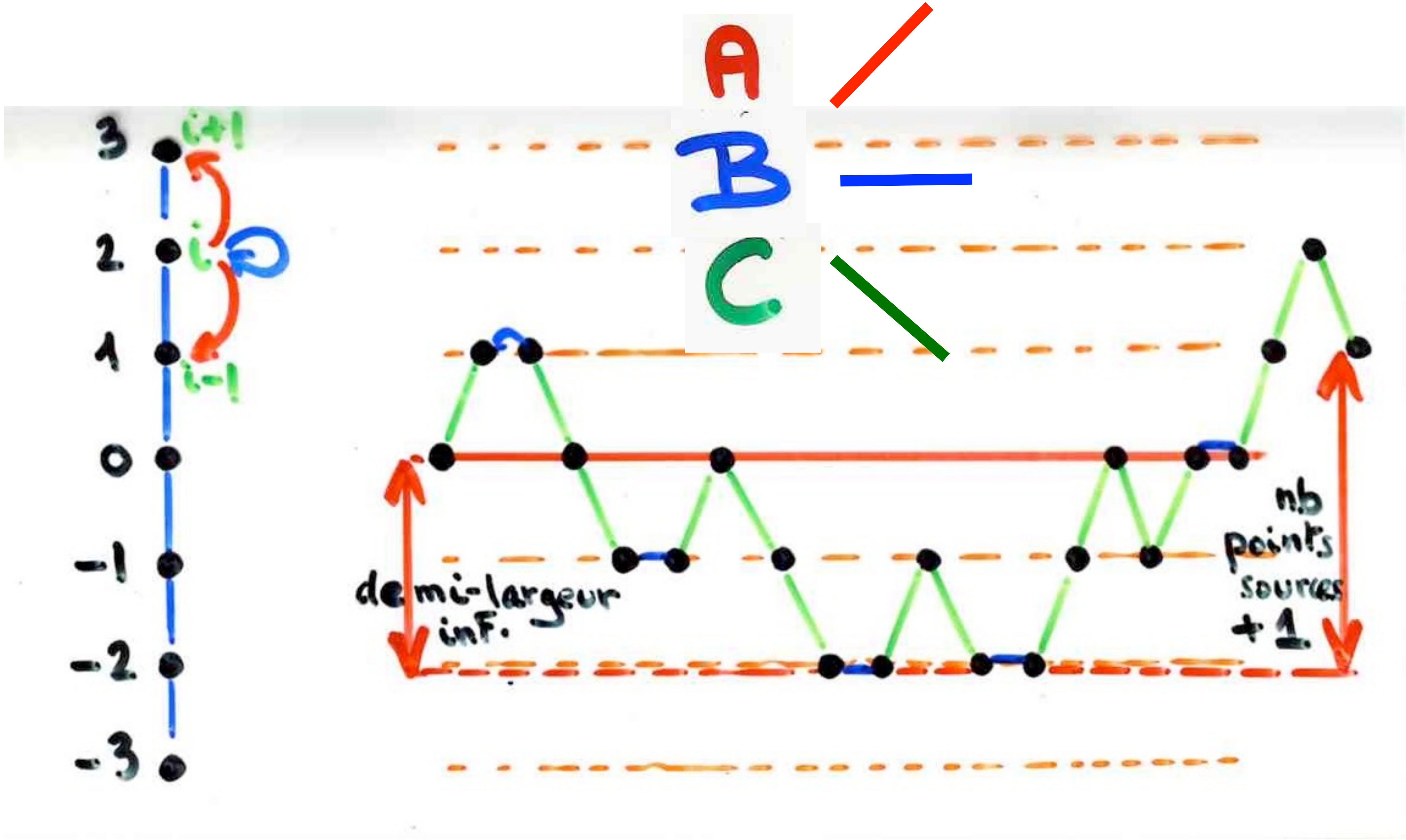
$$X = \frac{z}{1-3z}$$

J. Betrema

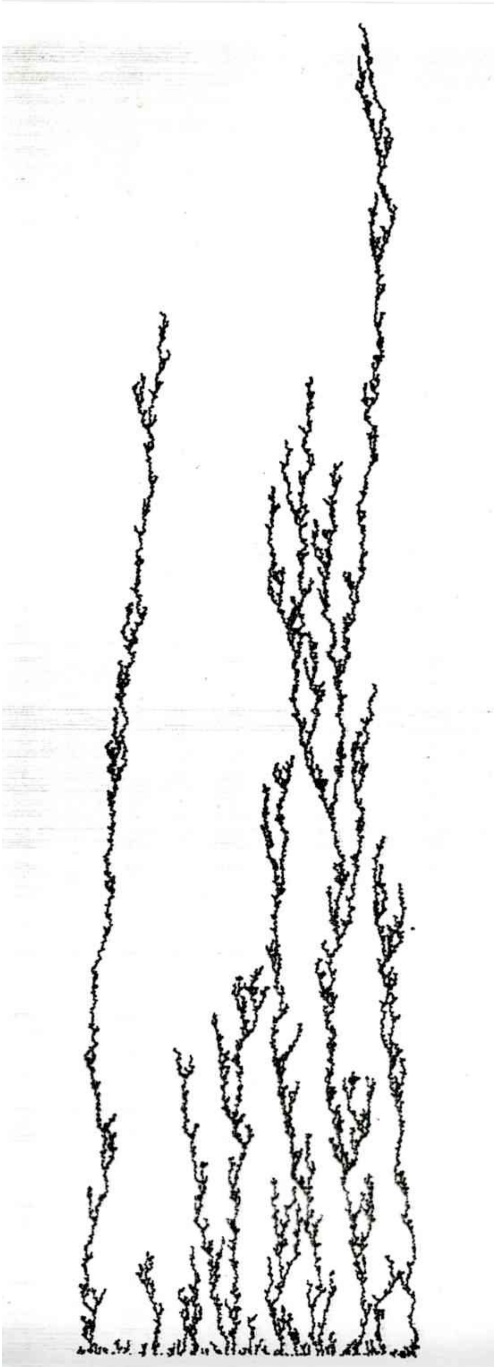
J.G. Penaud

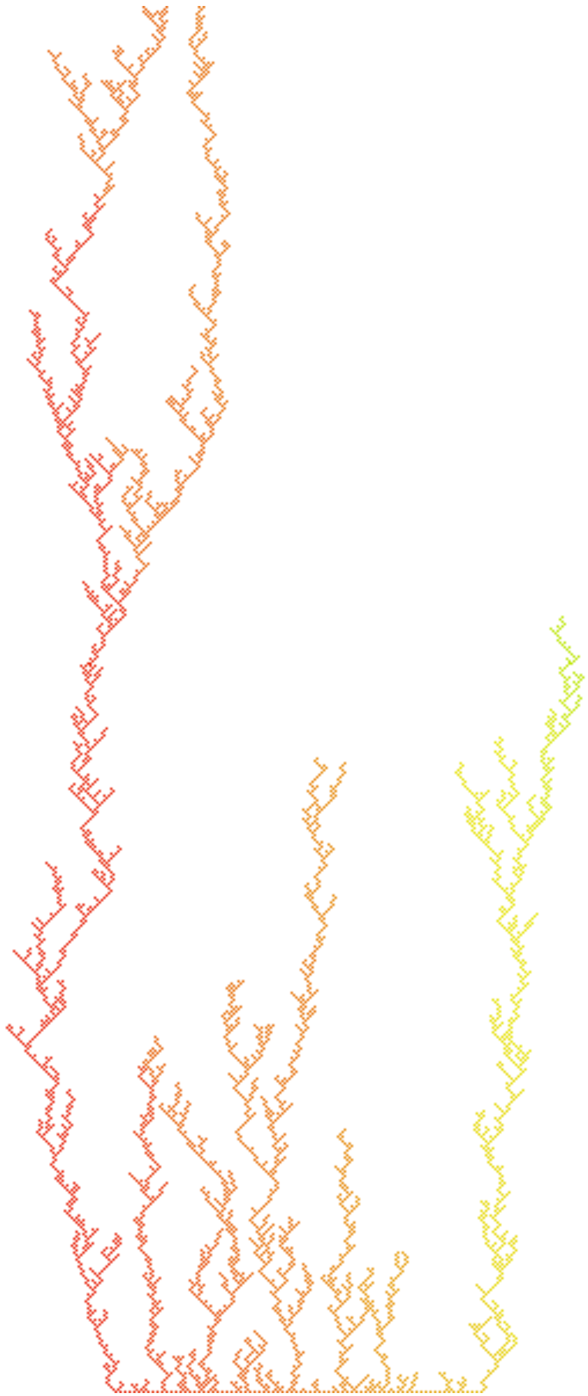
$$= z + 3z^2 + 3^2z^3 + \ldots + 3^n z^{n+1} + \ldots$$


$\ell_{inf} = 4$



D. Gouyou-Beauchamps
X. V. (1984)



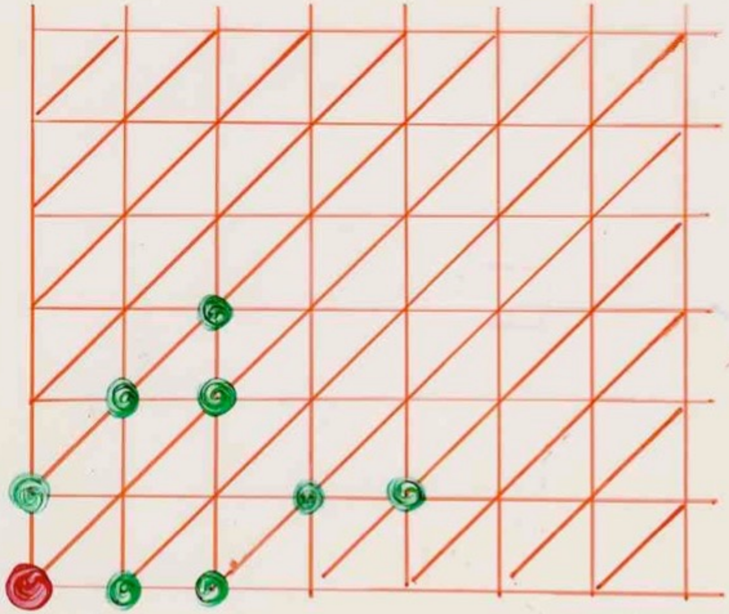


random

compact source
directed
animal

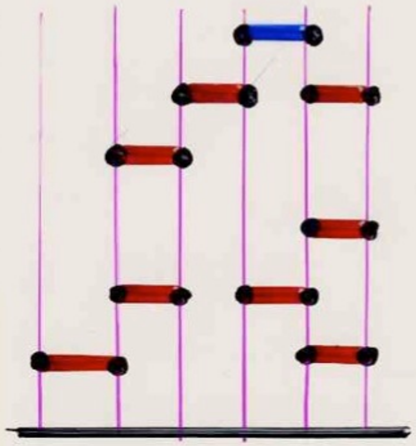
directed animals

on a triangular lattice



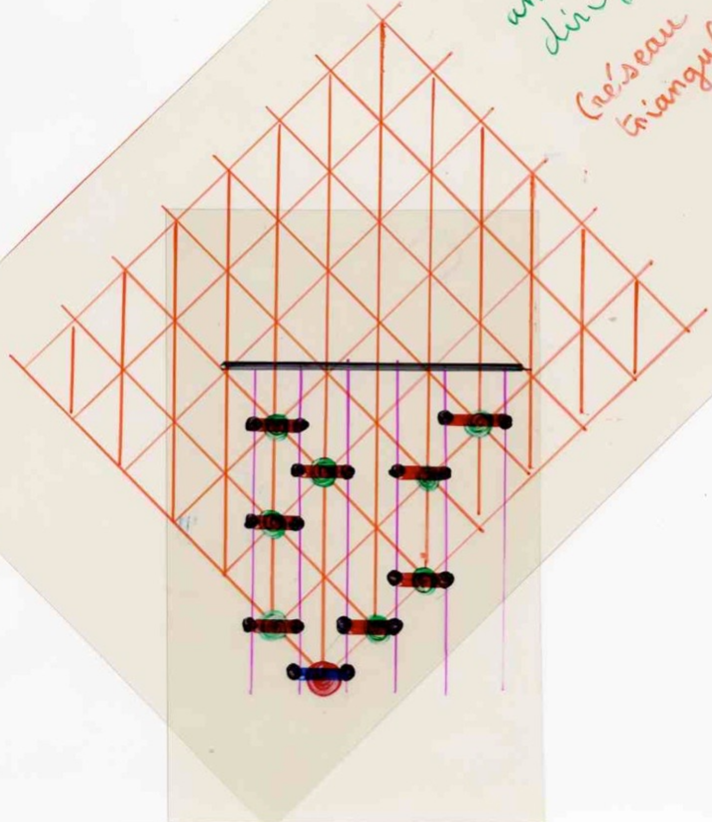
animal
dirigé
(réseau
triangulaire)

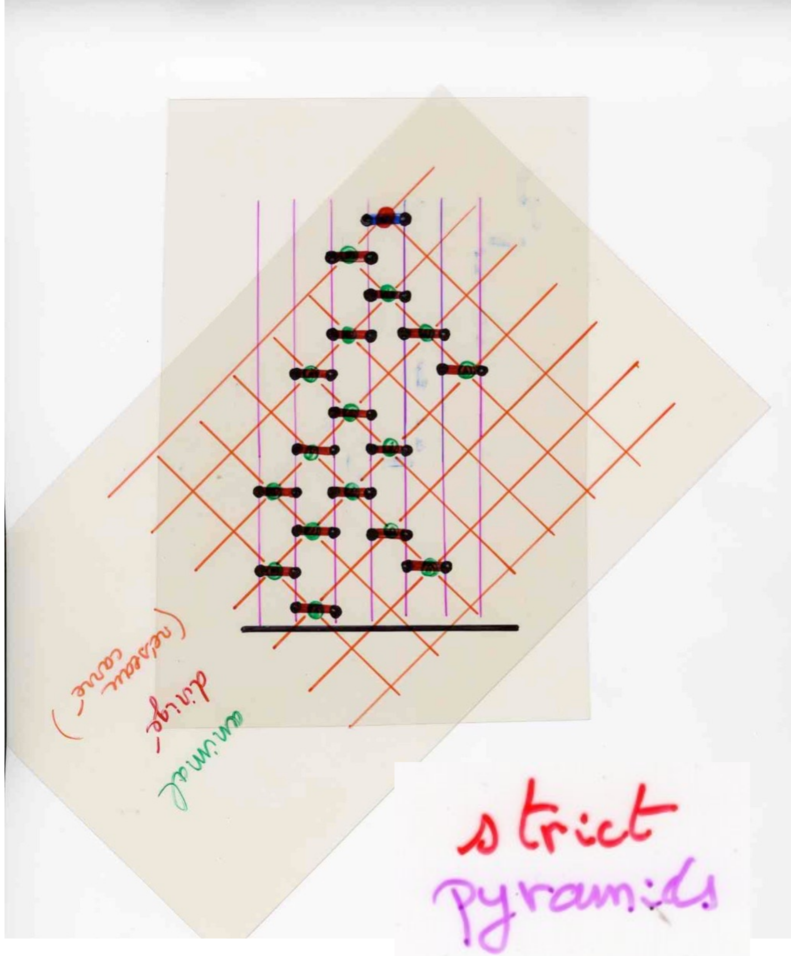
bijection



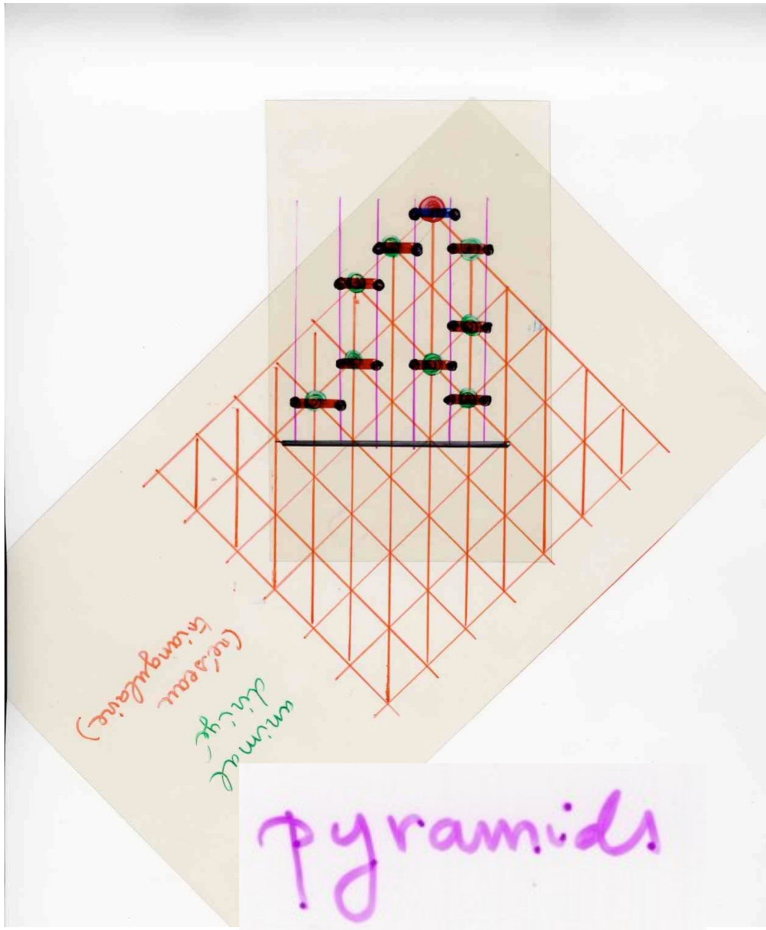
pyramids

directed
animal
(square
lattice)


animal
dirigé
(réseau
triangulaire)



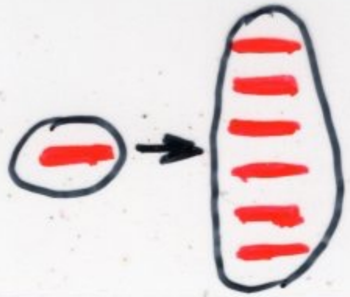
strict
pyramids



pyramids

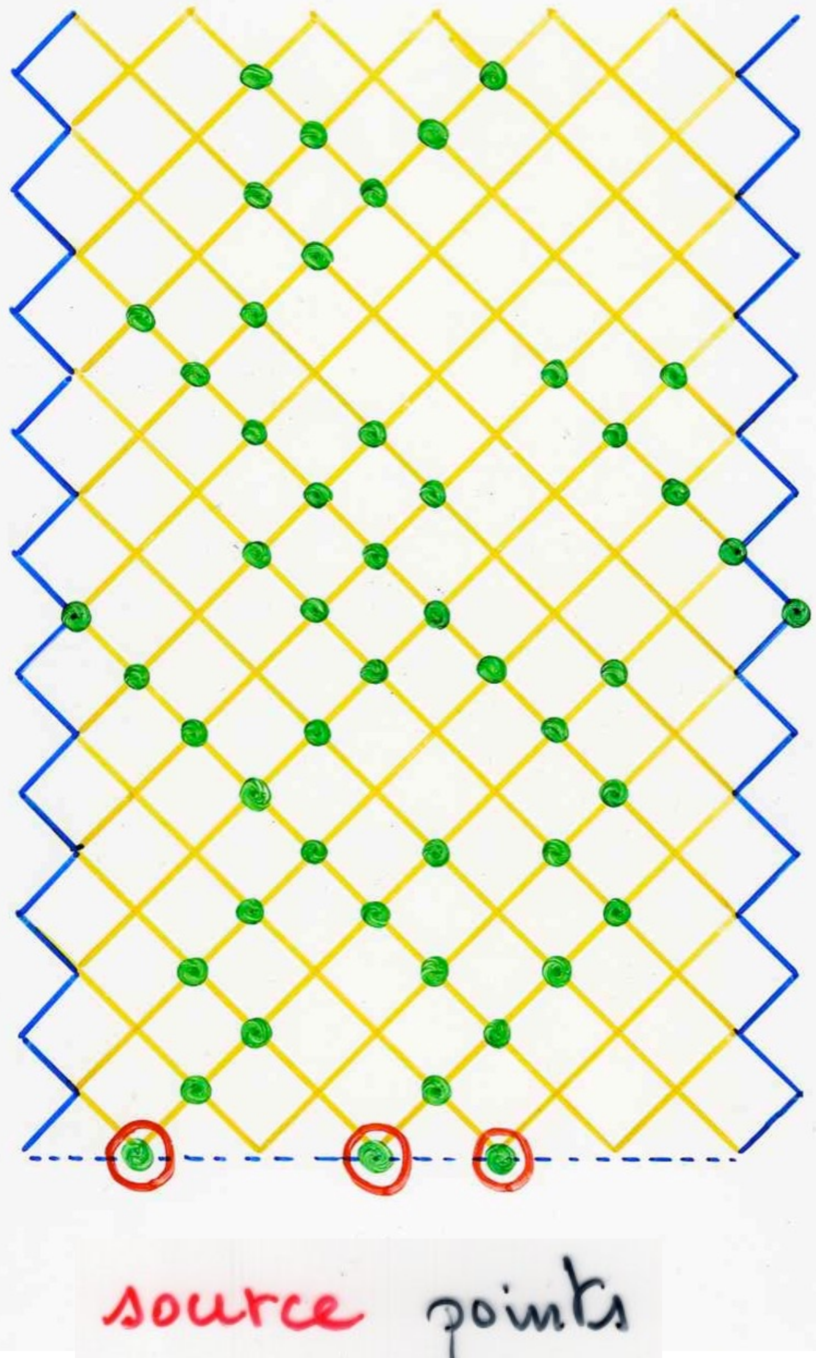
strict heap → heap

$$t \longrightarrow \frac{1}{1-t}$$



directed animals

on bounded strip



directed animal
on a circular strip

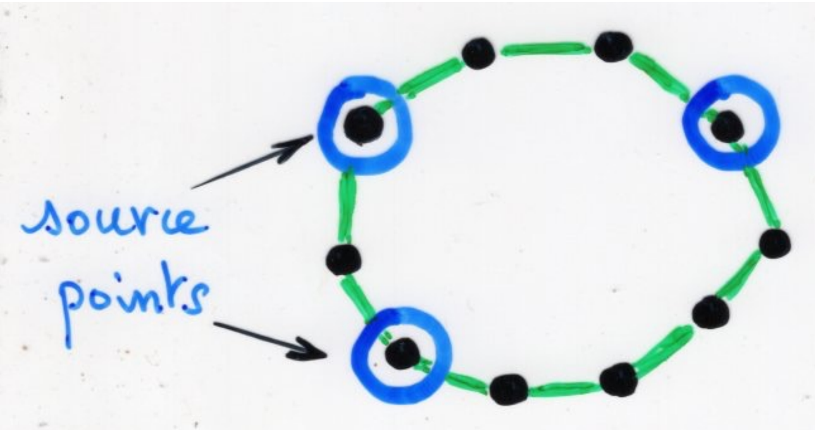
Nadal, Derrida, Vannimenus (1982)

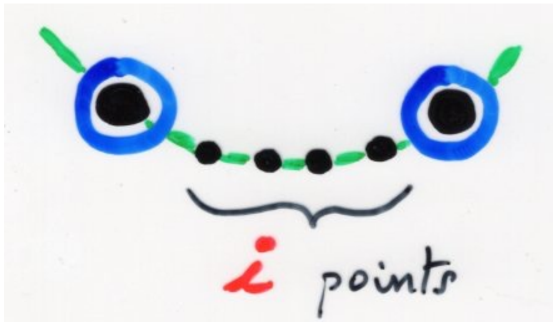
$$\tilde{b}_n^{\leq k} = \frac{1}{k} \sum_{p=0}^{k-1} (-1)^p \sin\alpha_p \prod_{i=1}^{k-1} \left(\frac{\sin(i+\frac{1}{2})\,\alpha_p}{\sin\frac{\alpha_p}{2}} \right)^{N_i} (1+2\cos\alpha_p)^{n-1}$$

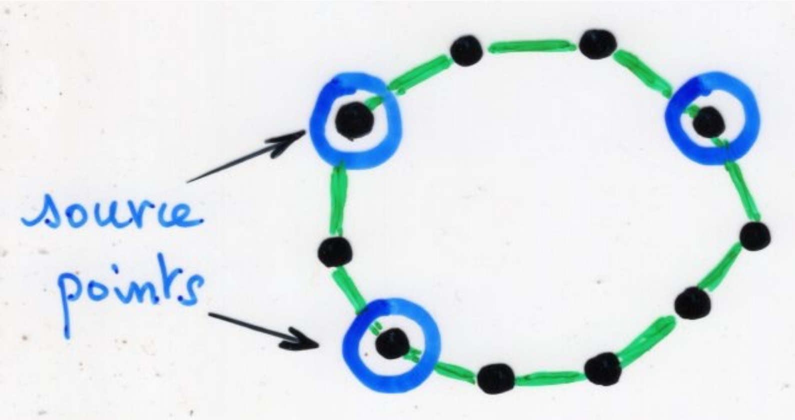
animals
circular strip
width k

$$\alpha_p = \frac{2p+1}{2k}\pi$$

N_i = number of i-holes







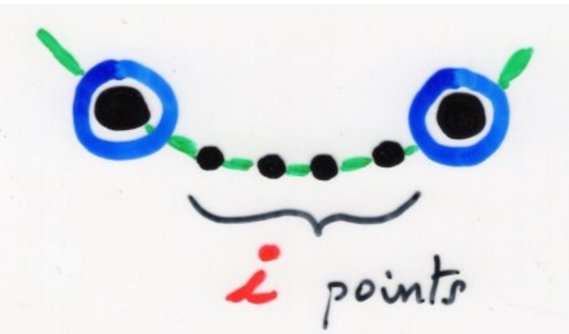
$$\frac{N}{D}$$

$$D = L_n(x)$$

Lucas polynomial

$$N = \prod_i F_i(x)$$

Fibonacci polynomial



N_i = number of i-holes

Nadal, Derrida, Vannimenus (1982)

$$\tilde{b}_n^{\leq k} = \frac{1}{k} \sum_{p=0}^{k-1} (-1)^p \sin\alpha_p \prod_{i=1}^{k-1} \left(\frac{\sin(i+\frac{1}{2})\alpha_p}{\sin\frac{\alpha_p}{2}} \right)^{N_i} (1+2\cos\alpha_p)^{n-1}$$

animals

circular strip

width k

$$\alpha_p = \frac{2p+1}{2k}\pi$$

$$\frac{N}{D} \qquad N = \prod_i F_i(x) \qquad D = L_n(x)$$

$$T_n(x) = \frac{1}{2} C_n(2x) \qquad C_n^* = L_n(x^2) \qquad \cos(n\theta) = T_n(\cos\theta)$$

zeros of $T_n(x)$: $\left\{ \cos\left(\frac{(2k-1)}{2n} \pi \right), \quad k = 1, .., n \right\}$

combinatorial understanding

of the thermodynamic limit

the case a 1D gas model

$$Z_n(t) = F_n(-t)$$

Fibonacci
polynomials

thermodynamic limit

$$\lim_{n\to\infty} \left(Z_n(t)\right)^{1/n}$$

$$\log Z_n^{1/n}(t) = \frac{1}{n} \log Z_n(t)$$

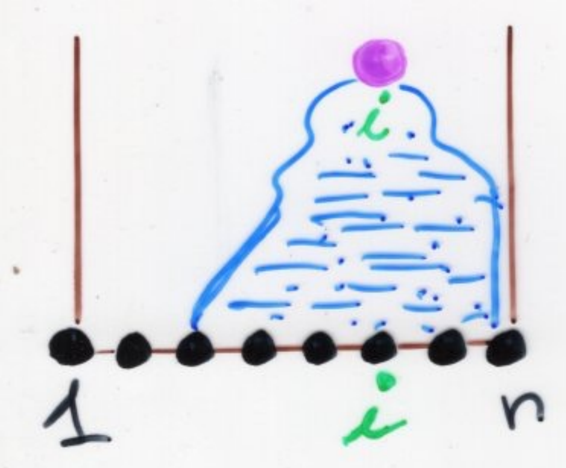
$$= -\frac{1}{n} \log \frac{1}{Z_n(t)}$$

$$-t \frac{d}{dt} \log Z_n^{1/n}(-t) = \underbrace{\frac{1}{n} t \frac{d}{dt} \log \frac{1}{Z_n(-t)}}_{\frac{1}{n} \mathrm{Pyr}_n(t)}$$

$\mathrm{Pyr}_n(t)$

generating function of pyramids on $[1,n]$

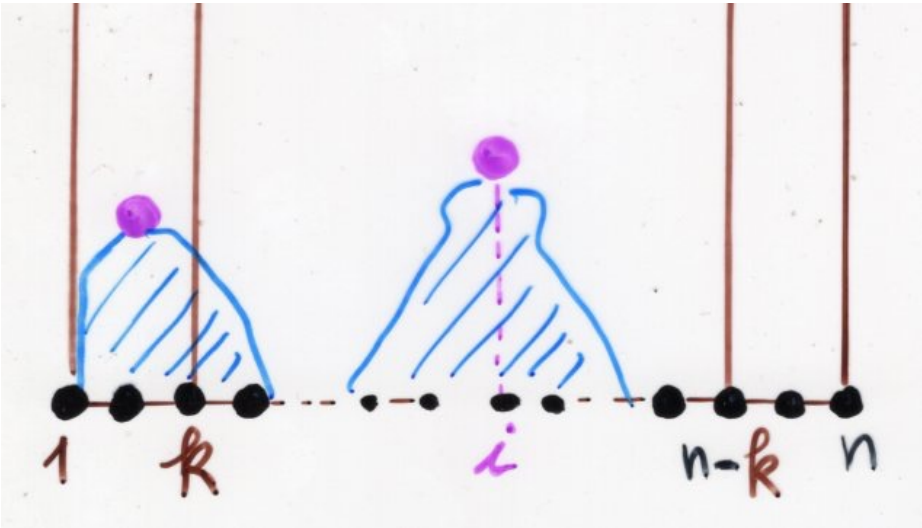
$$\mathrm{Pyr}_n(t) = \sum_{1 \le i \le n} \mathrm{Pyr}_n^i(t)$$



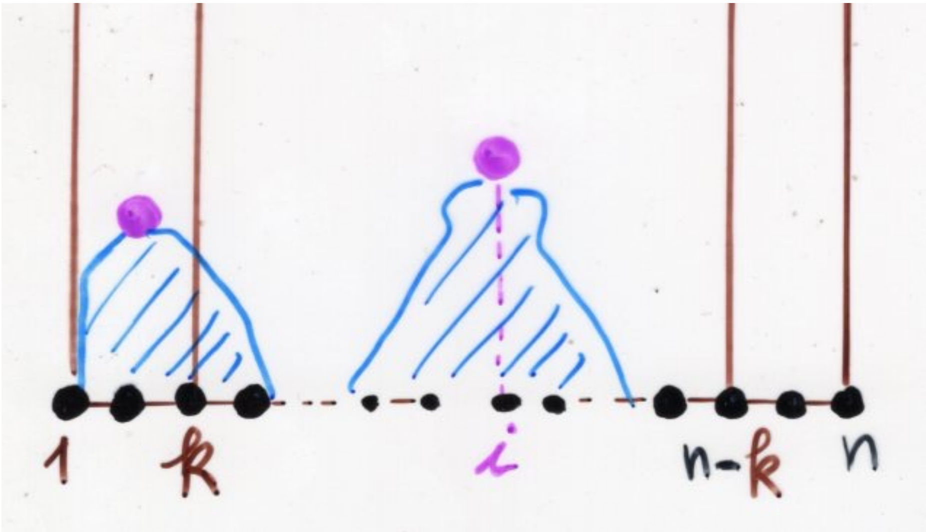
generating function of pyramids over $[1,n]$ with $\pi(\max) = i$

let $k \geq 1$

$$\mathrm{Pyr}^{i}_{n,k}(t) = t + a^{i}_{n,2}t^2 + \cdots + a^{i}_{n,k}t^k + \cdots$$



for $k \leq i \leq n-k$ $\mathrm{Pyr}^{i}_{n}(t)$ does not depend of i



$$\mathrm{Pyr}_{n,k}(t) = [n-2(k-1)]\,\mathrm{Pyr}^{*}_{n,k}(t) + \sum_{\substack{1\le i<k \\ \text{or } k<i\le n}} \mathrm{Pyr}^{i}_{n,k}$$

$$\frac{1}{n}\mathrm{Pyr}_{n,k}(t) = \left(1-\frac{2(k-1)}{n}\right)\mathrm{Pyr}^{*}_{n,k}(t) + \frac{1}{n}\sum_{\substack{1\le i<k \\ \text{or} \\ k<i\le n}} \mathrm{Pyr}^{i}_{n,k}(t)$$

k fixed
$n \to \infty$

$\longrightarrow 1$

$\longrightarrow 0$

define

$$\rho_n(t) = t\frac{d}{dt}\log Z_n(t)$$

$$\rho(t) = t\frac{d}{dt}\log Z(t)$$

density of the gas
t activity

$$\rho_n(t) \longrightarrow \rho(t)$$

means: for any k, the coefficients of the first k terms of $\rho_n(t) \longrightarrow$ coeff. of $\rho(t)$

density of the gas

t activity

$$\rho(t) = t\frac{d}{dt}\log Z(t)$$

$-\rho(-t)$ is the generating function of pyramids on $\mathbb{Z}$ (up to translation)

$$\frac{1}{2}\binom{2n}{n} \qquad \frac{1}{2}\frac{1}{\sqrt{1-4t}}$$

directed animals on the triangular lattice lattice

lattice

D.Dhar

equivalence
directed animal model
with
hard gas model

relation with
crystal growth model
stochastic lattice gas

$$Z(t) = \sum_{n \geq 0} b_n \frac{t^n}{n!}$$

b_n = nb of "assemblée" of signed labeled pyramids with (m)

(up to translation)

minimum label on the top piece

b_n divisible by $n!$?

research problem

$$\rho(t) = t\frac{d}{dt}\log Z(t)$$

$$Z(t) = 1 + t - 2t^2 + 5t^3 - 14t^4 + \dots + (-1)^{n+1} C_n + \dots$$

"assembleé"
of labeled pyramids
on $\mathbb{Z}$
(up to translation)
with condition (m)

Catalan number

$$C_n = \frac{1}{(n+1)}\binom{2n}{n}$$

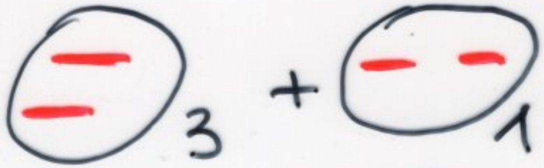
(the label of the maximal piece is the smallest) research problem

 1

assemblée

labeled

(m)

 $= 4 = 2 \times 2!$

$3 + 1 = 4 = 2 \times 2$

C_2 $2!$

Catalan

$10 = \frac{1}{2}\binom{6}{2}$ pyramids

3 dimers

10×2 labeling

3 pyr 3 labeling

$20 + 9 + 1 = 30$

$= 5 \times 6$

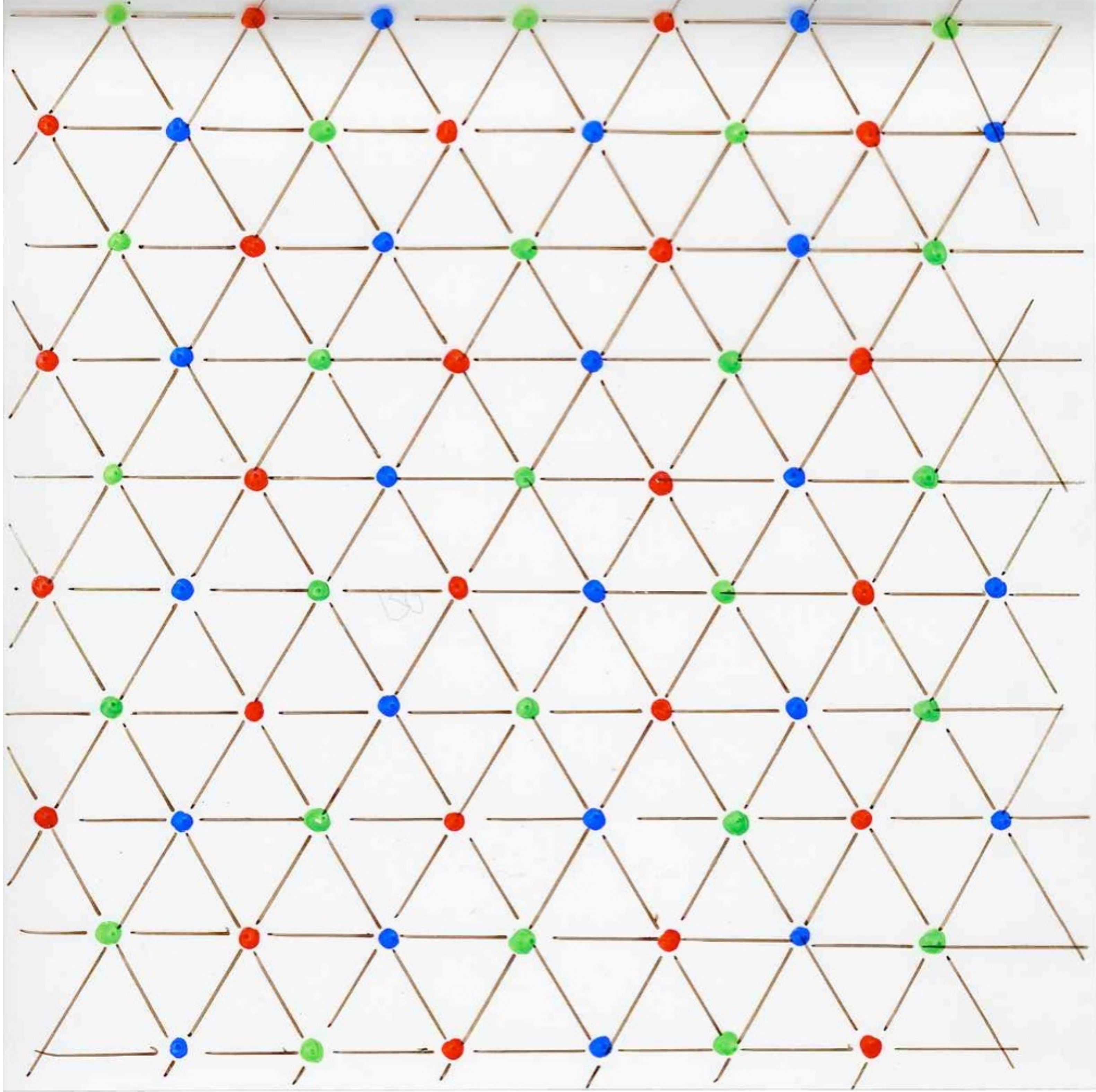
C_3 $3!$

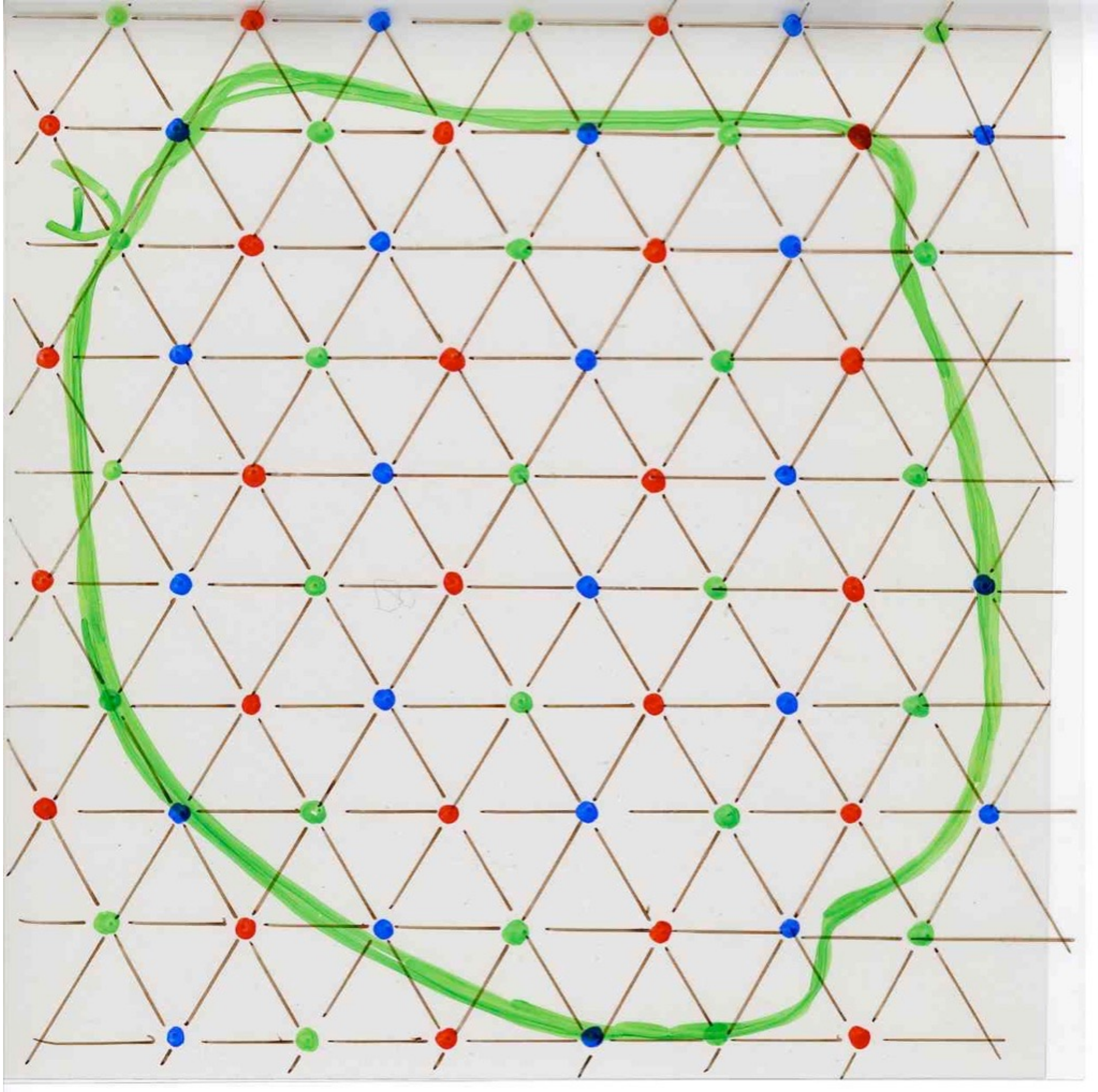
Catalan

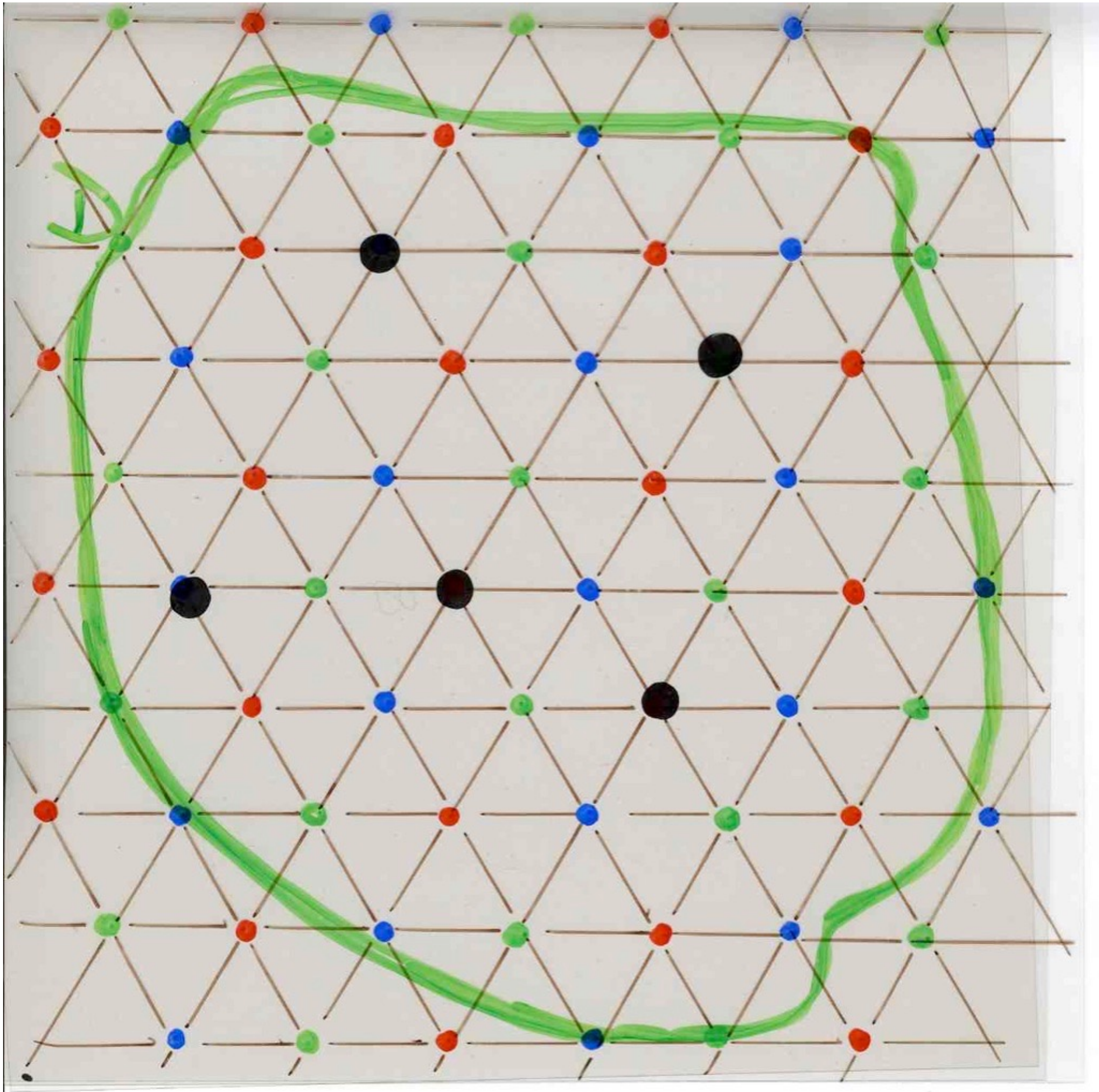
Hard Hexagons

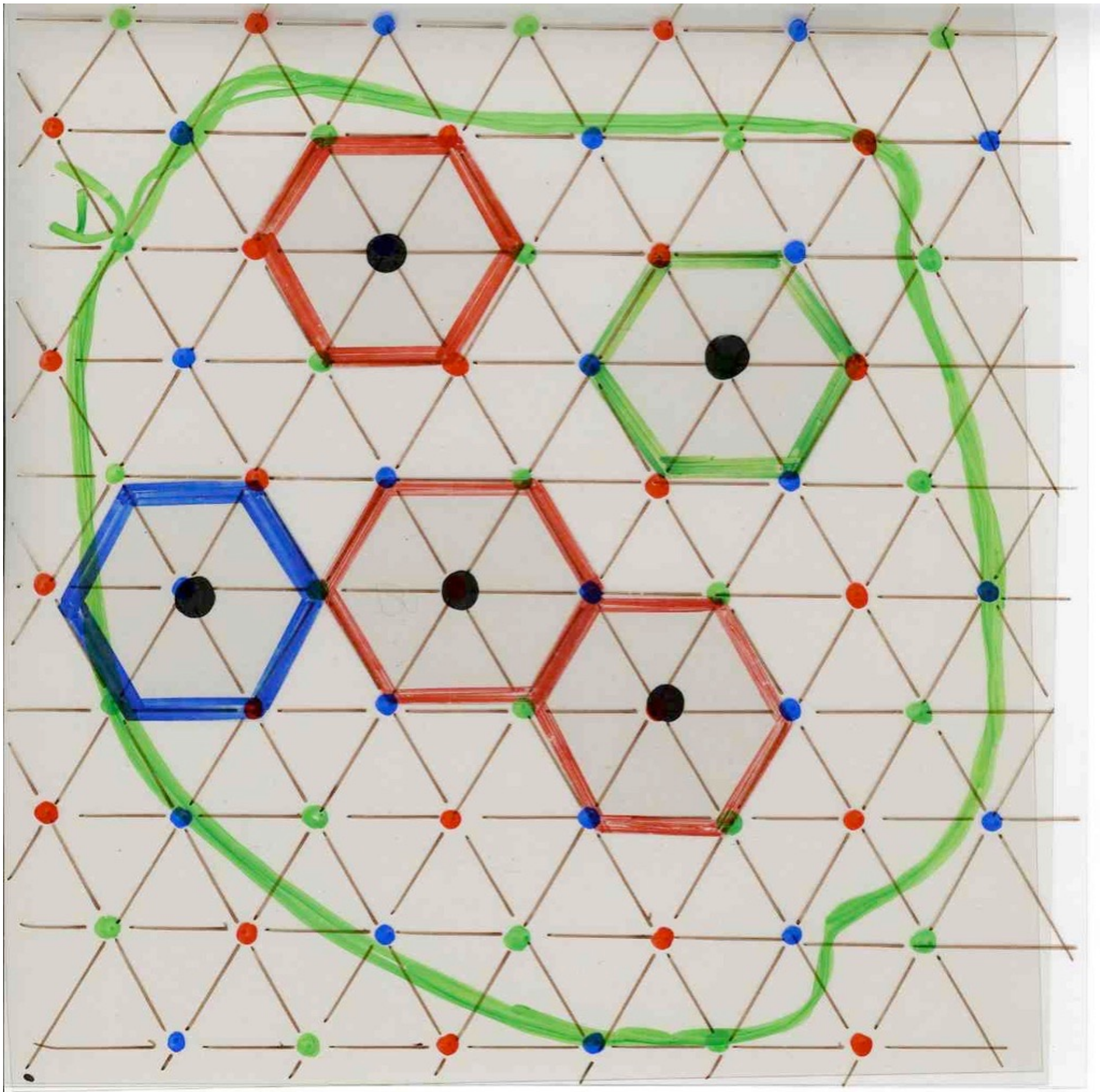
Baxter
1980
1982

gas model
with "hardcore interactions"









partition function

$$Z_D(t) = \sum_{n \geqslant 0} a_{n,D}\, t^n$$

$$Z(t) = \lim_{\text{"}D \to \infty\text{"}} \left(Z_D(t) \right)^{1/|D|}$$

thermodynamic limit

$$\rho(t) = t \frac{d}{dt} \log Z(t)$$

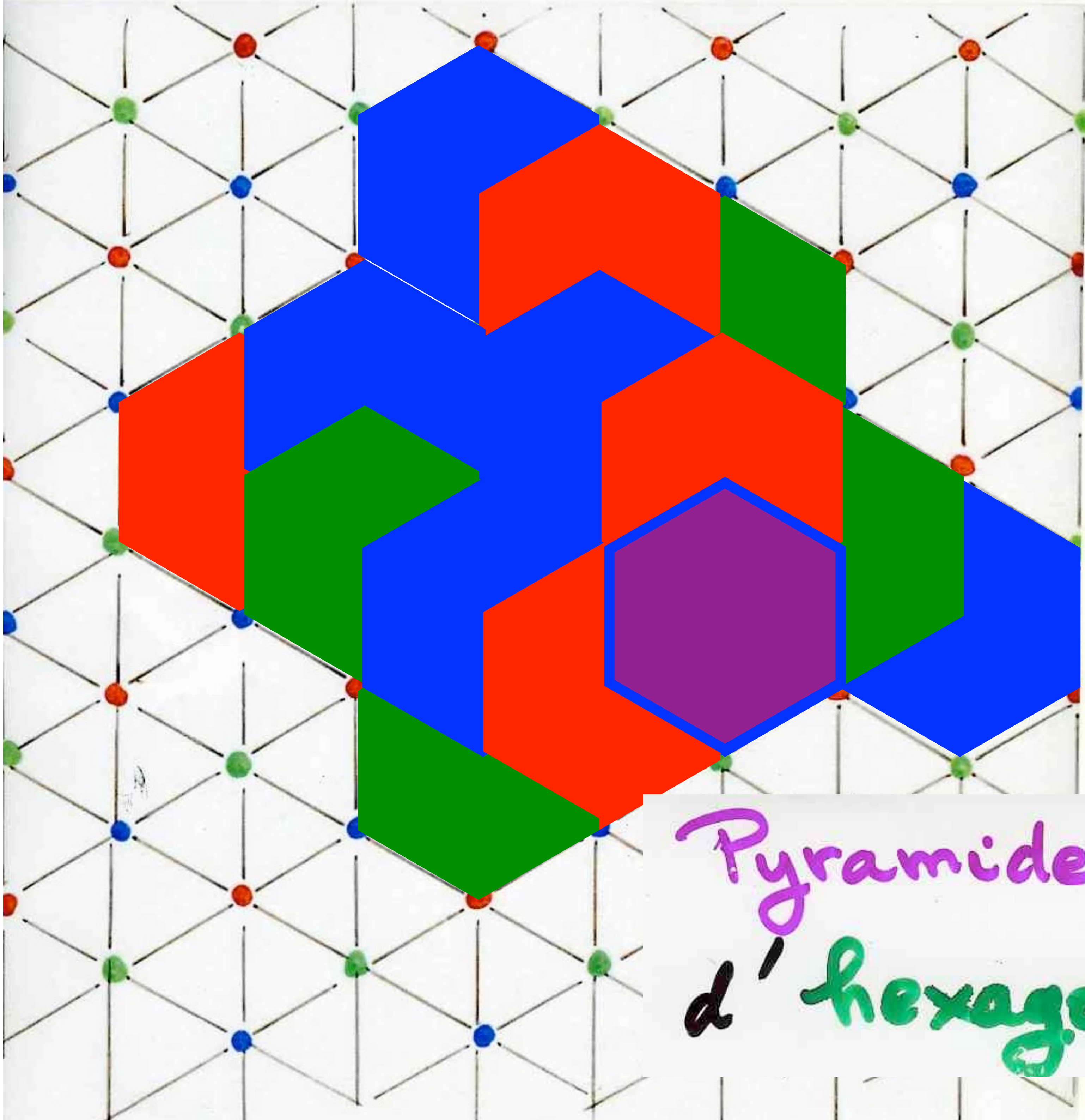
Proposition

$$-\rho(-t) = \sum_{n \geq 1} a_n t^n$$

density of the gas

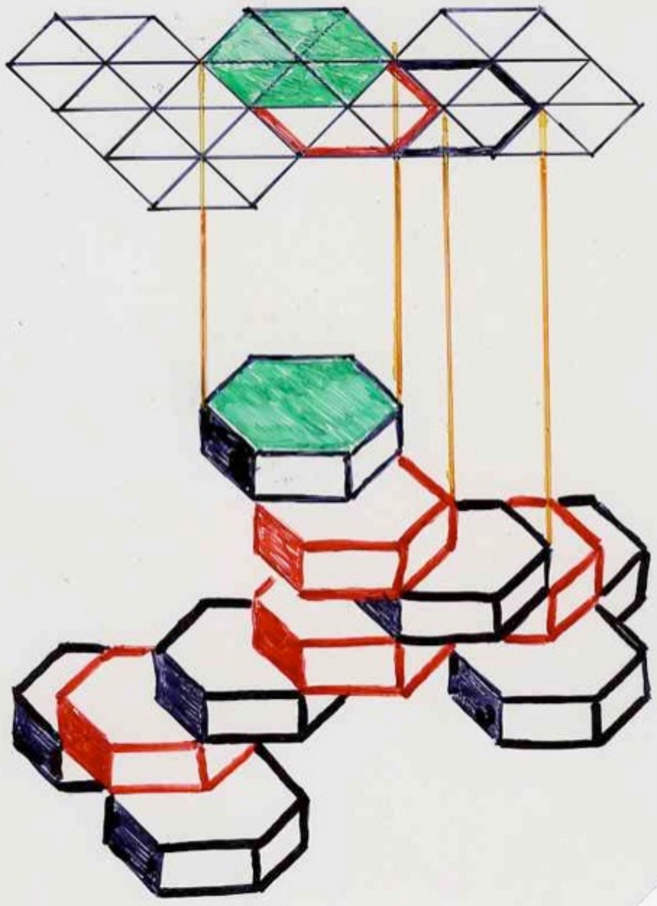
t activity

number of pyramids on the triangular lattice with n hexagons (up to translation)

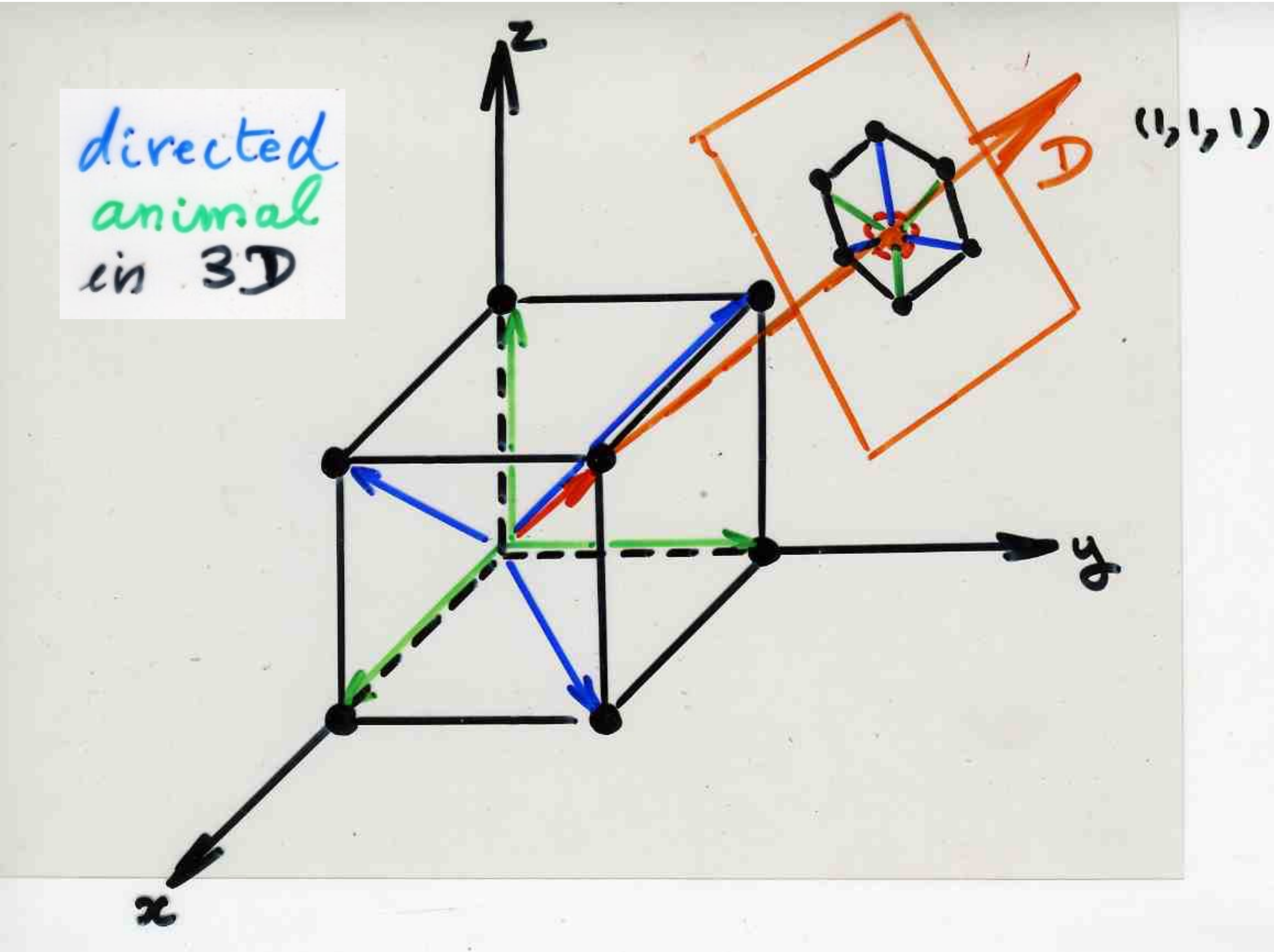


Pyramide d'hexagones

$$-p(-t) = y$$



HC.



directed
animal
in 3D
z
y
x
D
(1,1,1)

$$\rho(t) = t - 7t^2 + 58t^3 - 519t^4 + 4856t^5 - \cdots$$

combinatorial understanding

of the thermodynamic limit

the case of a 2D gas model

partition function

$$Z_D(t) = \sum_{n \geqslant 0} a_{n,D}\, t^n$$

$$Z(t) = \lim_{\text{"}D \to \infty\text{"}} \left(Z_D(t) \right)^{1/|D|}$$

thermodynamic limit

$$\rho(t) = t \frac{d}{dt} \log Z(t)$$

Proposition

$$-\rho(-t) = \sum_{n \geq 1} a_n t^n$$

number of pyramids on the triangular lattice with n hexagons (up to translation) proof

$\mathcal{D}$ finite domain of the triangular lattice

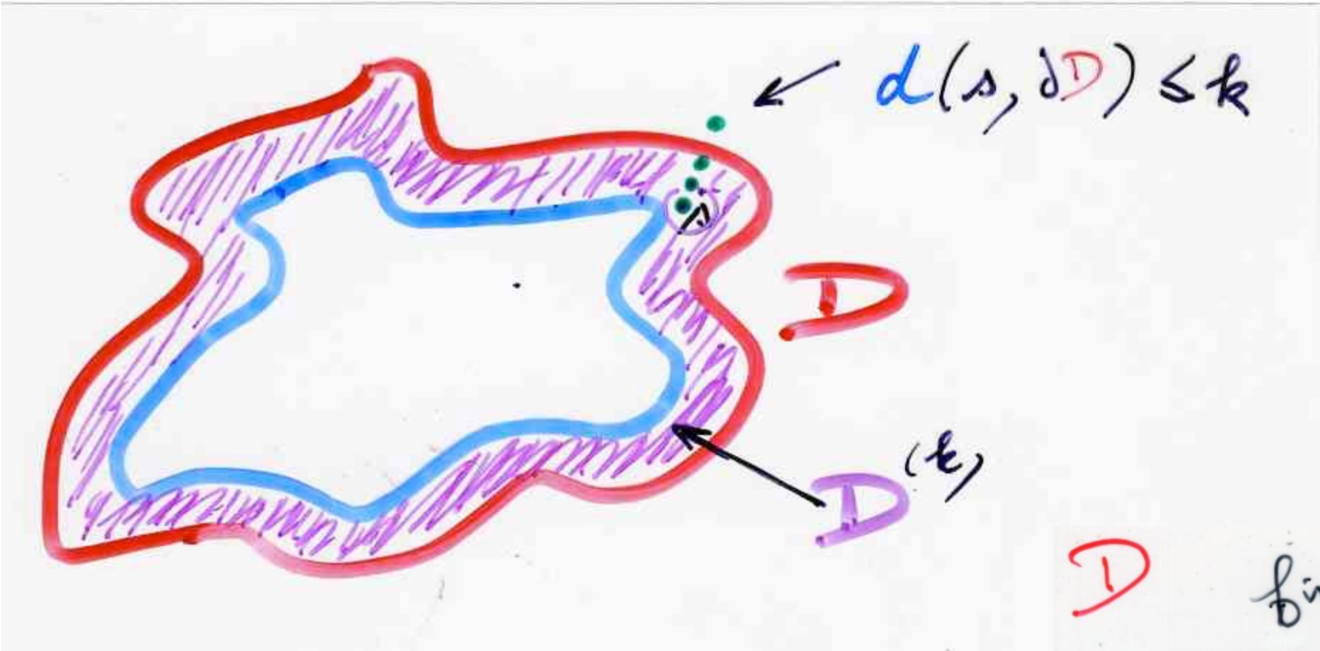
$s \in \mathcal{D}$ $\quad \mathbf{P}_{\mathcal{D},s}(t)$ generating function for pyramid

- projection in $\mathcal{D}$
- maximal piece s

Compute: $\displaystyle \frac{1}{|\mathcal{D}|} \sum_{s \in \mathcal{D}} \mathbf{P}_{\mathcal{D},s}(t) = \frac{1}{|\mathcal{D}|} \mathbf{P}_{\mathcal{D}}(t)$

Hexagon Pyramids on a tube of base $\mathcal{D}$

$$\mathbf{P}_{\mathcal{D}}(t) = (-t) \frac{d}{dt} \log Z_{\mathcal{D}}^{-1}(-t)$$



D finite domain of the triangular lattice

Def. $d(s,\partial D)$
smallest length of paths (on Hex) to go from s to the outside of D

$$D^{(k)} = \{ s \in D,\ d(s,\partial D) \leq k \}$$

Proposition

Sequence $D_1 \subseteq D_2 \subseteq \cdots D_n \subseteq$
such that for every k

$$\frac{|D_n^{(k)}|}{|D_n|} \to 0$$

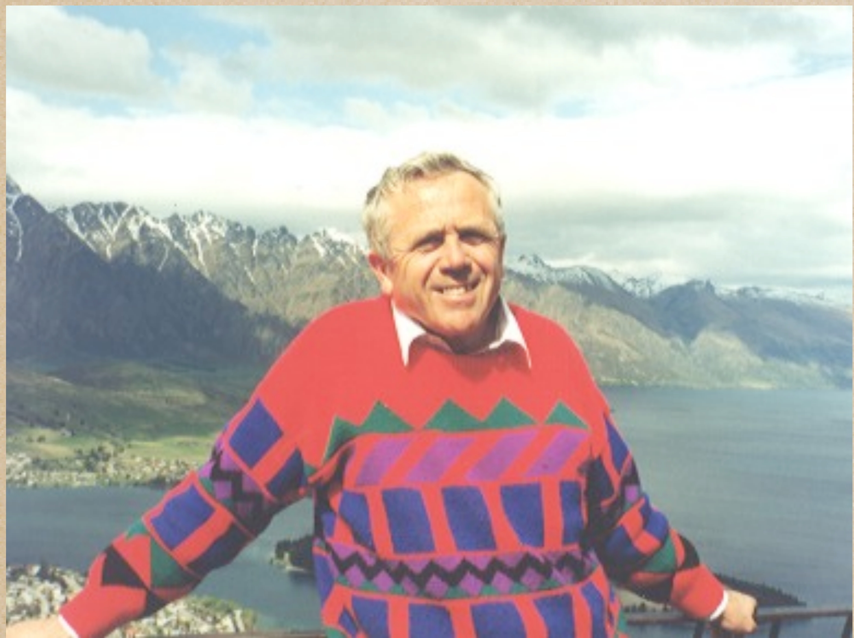
Then: $\frac{1}{|D_n|} \mathbf{P}_{D_n}(t) \to \mathbf{P}(t)$ generating function for Pyramid on Hex (up to translation)

means: $f_n(t) = \sum_{i \geq 0} a_{n,i} t^i$; $f(t) = \sum_{i \geq 0} a_i t^i$

then for every i, $a_{n,i} \to a_i$.

solution of the hard hexagons model

(R. Baxter, 1980)



Rogers - Ramanujan identities

R_{I}
$$\sum_{n\geq 0} \frac{q^{n^2}}{(1-q)(1-q^2)\cdots(1-q^n)} = \prod_{\substack{i\equiv 1,4 \\ \text{mod } 5}} \frac{1}{(1-q^i)}$$

R_{II}
$$\sum_{n\geq 0} \frac{q^{n^2+n}}{(1-q)(1-q^2)\cdots(1-q^n)} = \prod_{\substack{i\equiv 2,3 \\ \text{mod } 5}} \frac{1}{(1-q^i)}$$

"La fraction continue" de Ramanujan

$$\cfrac{1}{1+\cfrac{q}{1+\cfrac{q^2}{1+\cfrac{q^3}{\cfrac{\cdots}{1+\cfrac{q^k}{\cdots}}}}}} = \frac{\displaystyle\sum_{n\geq 0} \frac{q^{n^2+n}}{(1-q)(1-q^2)\cdots(1-q^n)}}{\displaystyle\sum_{n\geq 0} \frac{q^{n^2}}{(1-q)(1-q^2)\cdots(1-q^n)}}$$

$$R(q) = \prod_{n \geq 0} \frac{(1-q^{5n+1})(1-q^{5n+4})}{(1-q^{5n+3})(1-q^{5n+2})} = \frac{R_{II}}{R_{I}}$$

$$R(q) = \prod_{n \geqslant 0} \frac{(1-q^{5n+1})(1-q^{5n+4})}{(1-q^{5n+3})(1-q^{5n+2})} = \frac{R_{II}}{R_{I}}$$

$$t = -q\left[R(q)\right]^{5}$$

$$R(q) = \prod_{n\geq 0} \frac{(1-q^{5n+1})(1-q^{5n+4})}{(1-q^{5n+3})(1-q^{5n+2})} = \frac{R_{II}}{R_{I}}$$

$$t = -q\left[R(q)\right]^5$$

$$Y(q) = \prod_{n\geq 0} \frac{(1-q^{6n+2})(1-q^{6n+3})^2(1-q^{6n+4})(1-q^{5n+1})^2(1-q^{5n+4})^2(1-q^{5n})^2}{(1-q^{6n+1})(1-q^{6n+5})(1-q^{6n})^2(1-q^{5n+2})^3(1-q^{5n+3})^3}$$

$$R(q) = \prod_{n \geq 0} \frac{(1-q^{5n+1})(1-q^{5n+4})}{(1-q^{5n+3})(1-q^{5n+2})} = \frac{R_{II}}{R_{I}}$$

$$t = -q\left[R(q)\right]^5$$

$$Y(q) = \prod_{n \geq 0} \frac{(1-q^{6n+2})(1-q^{6n+3})^2(1-q^{6n+4})(1-q^{5n+1})^2(1-q^{5n+4})^2(1-q^{5n})^2}{(1-q^{6n+1})(1-q^{6n+5})(1-q^{6n})^2(1-q^{5n+2})^3(1-q^{5n+3})^3}$$

$$Z(t) = Y(q(t))$$

- critical temperature

$$T_c = \frac{11 + 5\sqrt{5}}{2}$$

- critical exponent $\frac{5}{6}$

$$= \left(\frac{1+\sqrt{5}}{2}\right)^{5}$$

$\frac{5}{6}$ critical exponent

Baxter

(1980)

$t_c = 11.09017..$

$\frac{1}{2}(11+5\sqrt{5})$

Gaunt 1967

critical temperature

for hexagons :

$(\phi)^5$

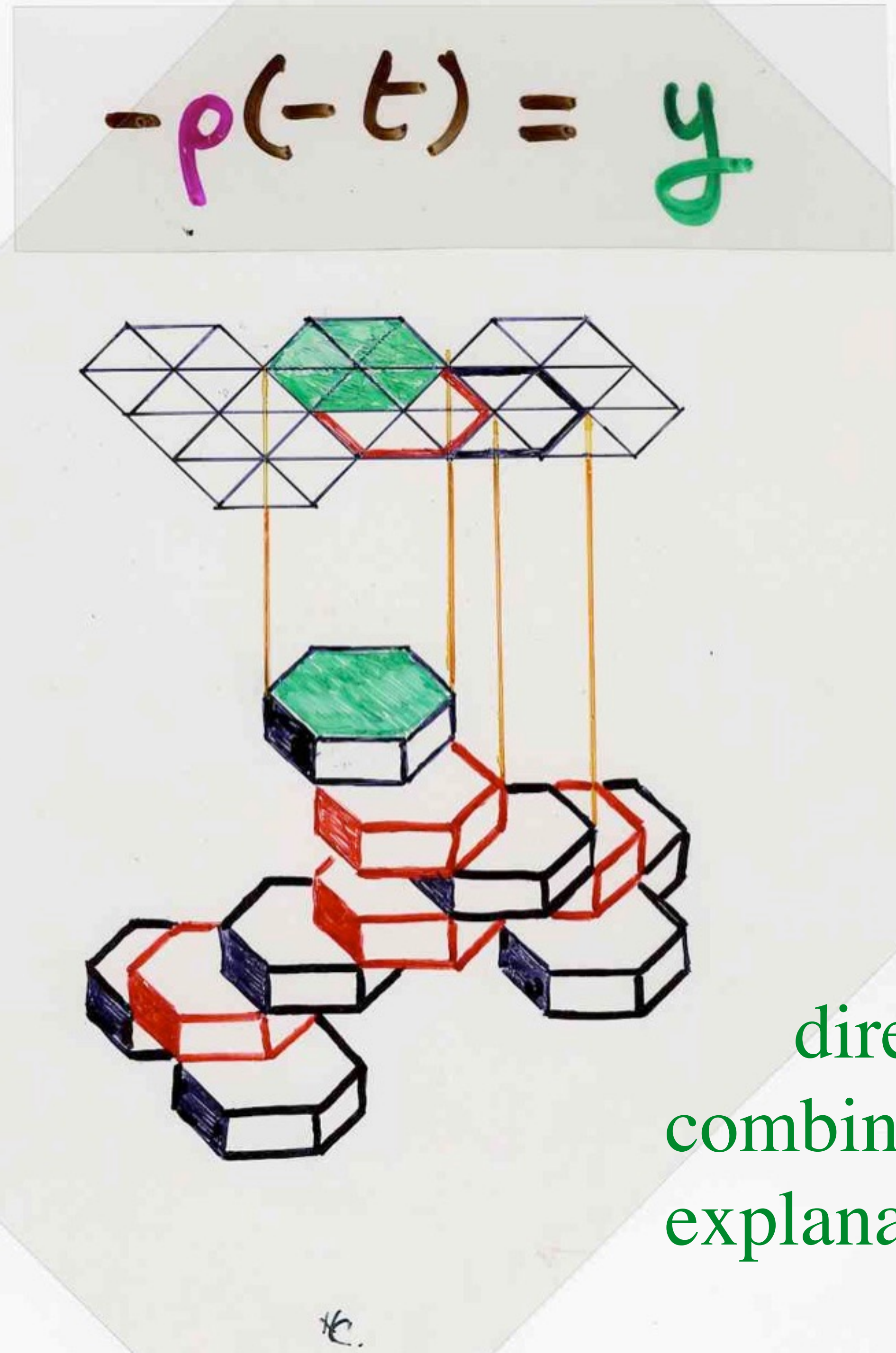
golden ratio

$$= \left(\frac{1+\sqrt{5}}{2}\right)^5$$

helium monolayer
absorbed onto
a graphite surface

(Riedel 1981)

research problem



algebraic
generating
function

direct
combinatorial
explanation ?

?

$$Z(t) = \sum_{n \geq 0} b_n \frac{t^n}{n!}$$

b_n = nb of "assemblée" of signed labeled pyramids with (*)

(up to translation)

(*) minimum label on the top piece

b_n divisible by $n!$?

$$Z(t) = 1 + t - 3t^2 + 16t^3 - 106t^4 + 789t^5 - 6318t^6 + \dots$$

Hard core
lattice gas models

interpretation of the density

hard square ?

algebraic
generating
function

?