

# Deterministic chaos, fractals and diffusion: From simple models towards experiments

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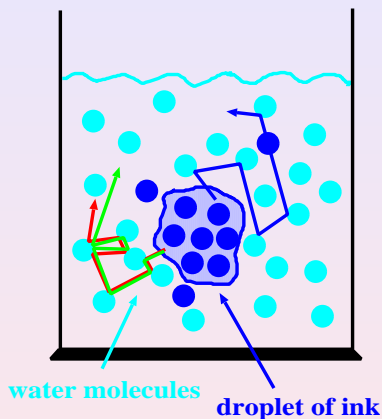
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# Outline

- 1 **Motivation:** random walks, diffusion and deterministic chaos
- 2 A simple model for **deterministic diffusion** with a **fractal diffusion coefficient**
- 3 From simple models towards experiments: **particle billiards** and **nanopores**

# Microscopic chaos in a glass of water?

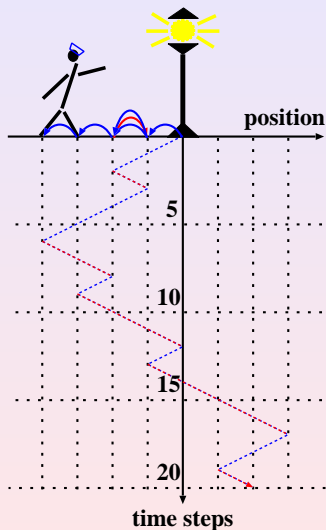


- dispersion of a droplet of ink by *diffusion*
- assumption: *chaotic collisions* between billiard balls

**microscopic chaos**  
 $\updownarrow$   
**macroscopic transport**

J.Ingenhousz (1785), R.Brown (1827), L.Boltzmann (1872),  
 P.Gaspard et al. (Nature, 1998)

# The drunken sailor at a lamppost



## simplification:

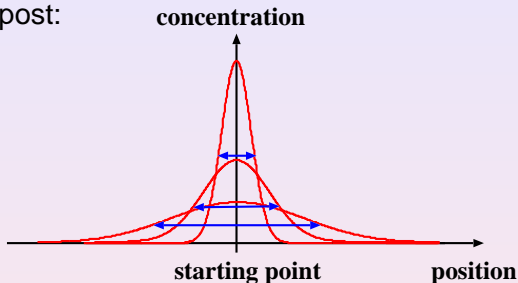
random walk in one dimension:

- steps of *length*  $s$  to the left/right
- sailor is **completely drunk**, i.e., the steps are *uncorrelated* (cp. to coin tossing)

K. Pearson (1905)

# The diffusion coefficient

consider a **large number** (ensemble) of sailors starting from the same lamppost:



define the **diffusion coefficient** by the **width** of the distribution: it is a **quantitative measure** of **how quickly** a droplet spreads out

$$D := \lim_{n \rightarrow \infty} \frac{\langle x^2 \rangle}{2n} \quad \text{with} \quad \langle x^2 \rangle := \int dx x^2 \rho_n(x)$$

as the *second moment* of the particle density  $\rho$  at time step  $n$

A. Einstein (1905)

# Basic idea of deterministic chaos

drunken sailor with **memory**? modeling by **deterministic chaos**

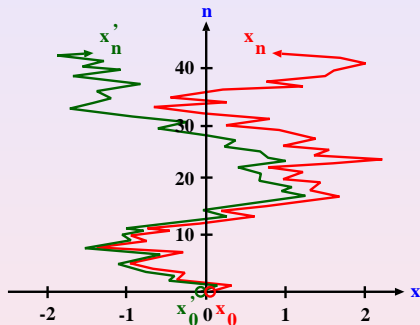
simple equation of motion

$$x_{n+1} = M(x_n)$$

for position  $x \in \mathbb{R}$

at discrete time  $n \in \mathbb{N}_0$

with **chaotic map**  $M(x)$



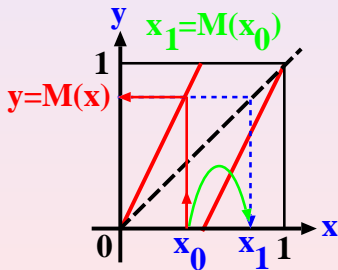
- the starting point **determines** where the sailor will move
- **sensitive dependence** on initial conditions

# Dynamics of a deterministic map

**goal:** study **diffusion** on the basis of **deterministic chaos**

**key idea:** replace **stochasticity** of drunken sailor by **chaos**  
**why?** **determinism** preserves all **dynamical correlations!**

model a single step by a **deterministic map:**



steps are iterated in discrete time  
 according to the equation of motion

$$x_{n+1} = M(x_n)$$

with

$$M(x) = 2x \bmod 1$$

**Bernoulli shift**

# Quantifying chaos: Ljapunov exponents

Bernoulli shift dynamics again:  $x_n = 2x_{n-1} \bmod 1$

what happens to small perturbations  $\Delta x_0 := x'_0 - x_0 \ll 1$ ?

use equation of motion:  $\Delta x_1 := x'_1 - x_1 = 2(x'_0 - x_0) = 2\Delta x_0$

iterate the map:

$$\Delta x_n = 2\Delta x_{n-1} = 2^2\Delta x_{n-2} = \dots = 2^n\Delta x_0 = e^{n \ln 2} \Delta x_0$$

$\lambda := \ln 2$ : **Ljapunov exponent**; A.M.Ljapunov (1892)

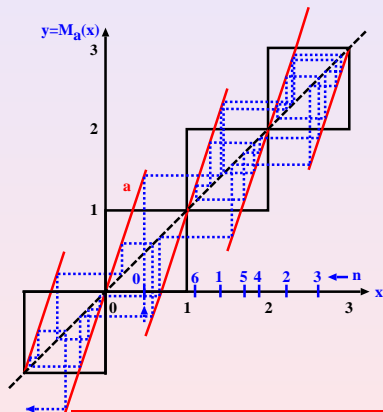
rate of **exponential growth** of an initial perturbation

here  $\lambda > 0$ : Bernoulli shift is **chaotic**



# A deterministically diffusive model

continue the Bernoulli shift on a **periodic lattice** by *coupling* the single cells with each other; Grossmann, Geisel, Kapral (1982):



$$x_{n+1} = M_a(x_n)$$

equation of motion for **non-interacting point particles** moving through an array of identical scatterers

slope  $a \geq 2$  is a **parameter** controlling the step length

**challenge:** calculate the **diffusion coefficient**  $D(a)$

# Computing deterministic diffusion coefficients

rewrite Einstein's formula for the diffusion coefficient as

$$D_n(a) = \frac{1}{2} \langle v_0^2 \rangle + \sum_{k=1}^n \langle v_0 v_k \rangle \rightarrow D(a) \quad (n \rightarrow \infty)$$

## Taylor-Green-Kubo formula

with velocities  $v_k := x_{k+1} - x_k$  at discrete time  $k$  and equilibrium density average  $\langle \dots \rangle := \int_0^1 dx \varrho_a(x) \dots$ ,  $x = x_0$

**1. inter-cell dynamics:**  $T_a(x) := \int_0^x d\tilde{x} \sum_{k=0}^{\infty} v_k(\tilde{x})$  defines fractal functions  $T_a(x)$  solving a (de Rham-) functional equation

**2. intra-cell dynamics:**  $\varrho_a(x)$  is obtained from the Liouville equation of the map on the unit interval

**structure of formula:**

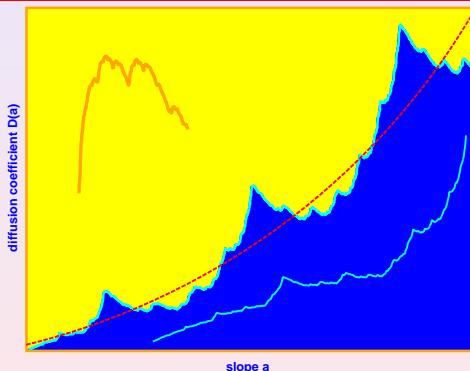
first term yields **random walk**, others higher-order **correlations**

see, e.g., Knight, R.K., Nonlinearity and PRE (2011)

# Parameter-dependent deterministic diffusion

exact analytical results for this model:

$D(a)$  exists and is a **fractal function of the control parameter**

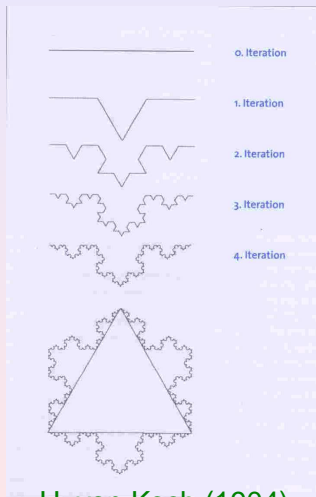


compare diffusion of drunken sailor with chaotic model:

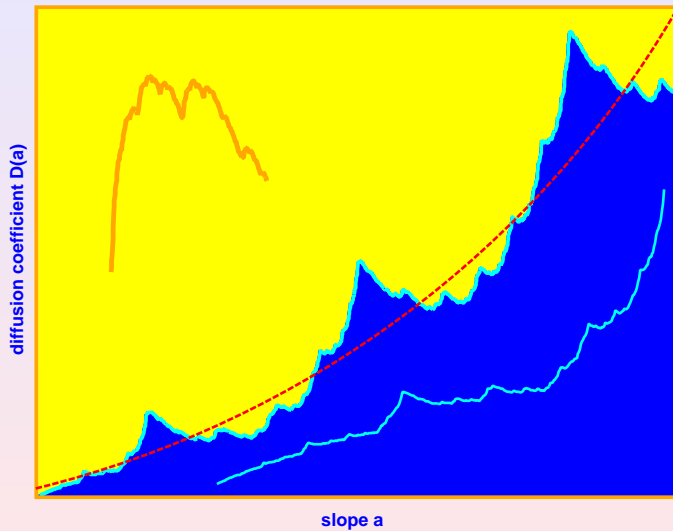
⊃ **fine structure beyond simple random walk solution**

R.K., Dorfman, PRL (1995)

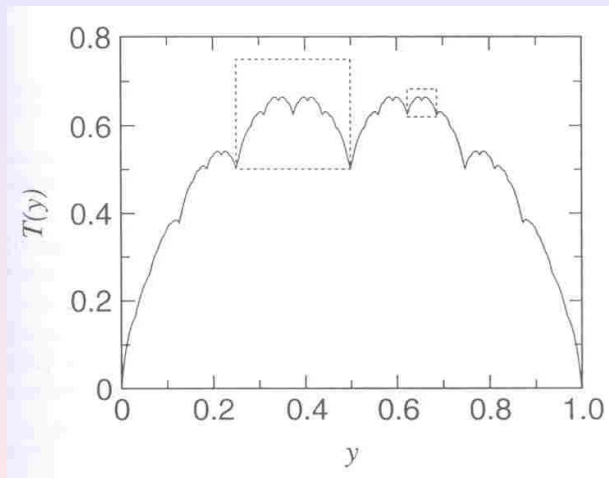
# Fractals 1: von Koch's snowflake



H. von Koch (1904)

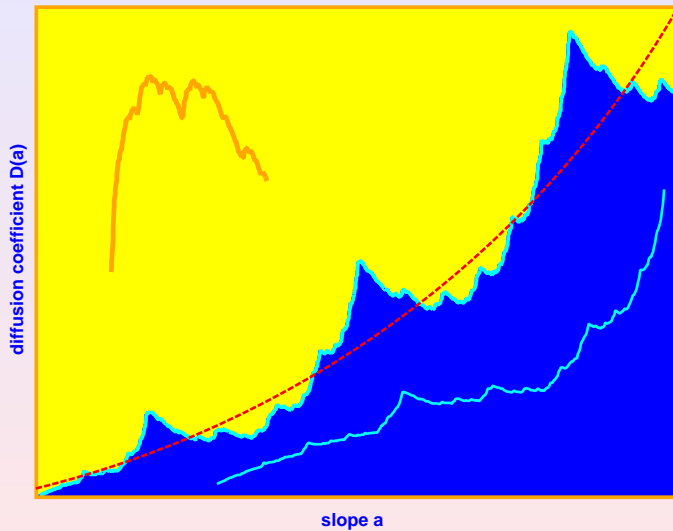


# Fractals 2: the Takagi function

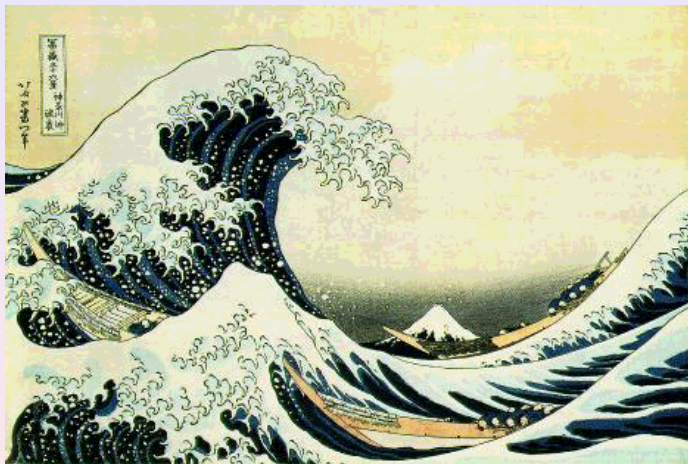


T.Takagi (1903)

example of a **continuous but nowhere differentiable function**



# 'Fractals 3': art meets science

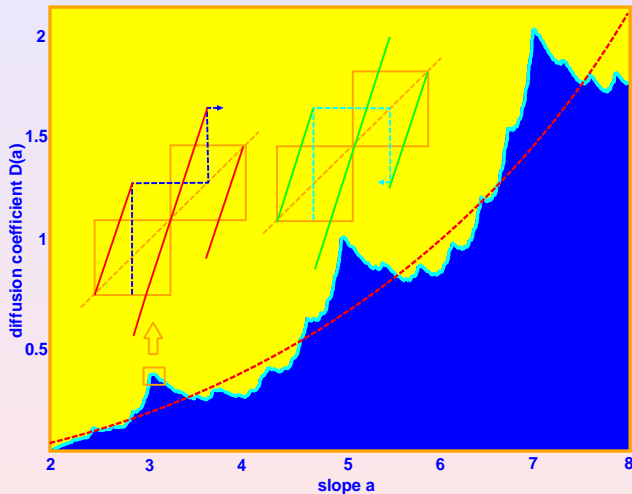


K.Hokusai (1760-1849)

*The great wave of Kanagawa; woodcut*



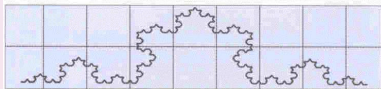
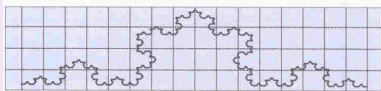
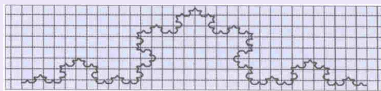
# Physical explanation of the fractal structure



local extrema are related to specific sequences of (higher order) **correlated microscopic scattering processes**

# Quantify fractals: fractal dimension

**example:** von Koch's curve; define a 'grid of boxes'



- count the number of boxes  $N$  covering the curve
- reduce the box size  $\epsilon$
- **assumption:**  $N \sim \epsilon^{-d}$

$$d = -\ln N / \ln \epsilon \quad (\epsilon \rightarrow 0)$$

**box counting dimension**

- can be **integer**:  
point:  $d = 0$ ; line:  $d = 1$ ; ...
  - can be **fractal**:  
von Koch's curve:  $d \simeq 1.26$   
Takagi function:  $d = 1$  !  
diffusion coefficient:  $d = 1$  but  
 $N(\epsilon) = C_1 \epsilon^{-1} (1 + C_2 \ln \epsilon)^\alpha$   
with  $0 \leq \alpha \leq 1.2$  **locally varying**
- Keller, Howard, R.K. (2008)

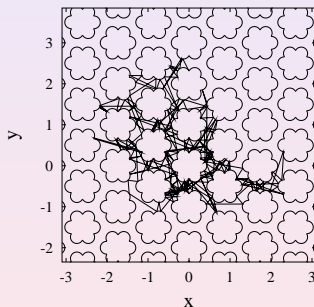
# The flower-shaped billiard

deterministic diffusion in physically more realistic models:

## Hamiltonian particle billiards

**example:**

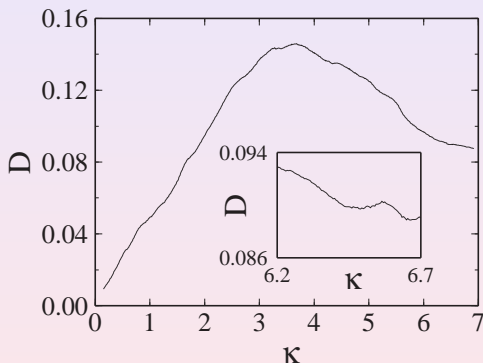
**flower-shaped hard disks** on a two-dimensional periodic lattice  
moving **point particles** collide elastically with the disks *only*:  
**Knudsen diffusion (1909)**



similar settings for electrons in semiconductor **antidot lattices**,  
**cold atoms in optical lattices**, and diffusion in **porous media**

# Diffusion in the flower-shaped billiard

**diffusion coefficient** as a function of the curvature  $\kappa = 1/R$  of the petals from simulations:



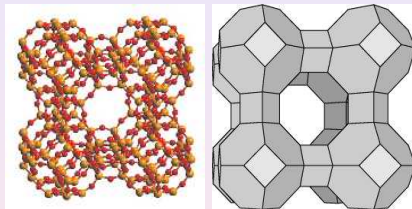
again a non-monotonic function of the control parameter with **irregular structure on fine scales**

Harayama, R.K., Gaspard (2002)

# Molecular diffusion in zeolites

**zeolites:** nanoporous crystalline solids serving as molecular sieves, adsorbants; used in detergents and as catalysts for oil cracking

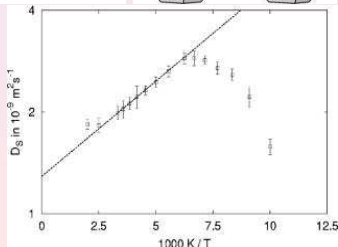
**example:** unit cell of **Linde type A zeolite**; strictly periodic structure built by a “cage” of silica and oxygen



**Schüring et al. (2002):** MD simulations with ethane yield **non-monotonic temperature dependence** of diffusion coefficient

$$D(T) = \lim_{t \rightarrow \infty} \frac{\langle [\mathbf{x}(t) - \mathbf{x}(0)]^2 \rangle}{6t}$$

due to **dynamical correlations**



# Summary

- **central theme:**  
relevance of **microscopic deterministic chaos** for **diffusion in periodic lattices**
- **main theoretical finding:**  
existence of diffusion coefficients that are **irregular (fractal) functions under parameter variation**, due to *memory effects* expected to be **typical** for classical transport in **low-dimensional, spatially periodic** systems
- **open question:** clearcut verification in **experiments?** good candidates: **nanopores, electronic transport in nanostructures, Josephson junctions, vibratory conveyors**

# Acknowledgements and literature

## work performed with:

J.R.Dorfman (College Park, USA), P.Gaspard (Brussels),  
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## literature:

