

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

Rainer Klages

Queen Mary University of London, School of Mathematical Sciences

Institut für Laserphysik, Universität Hamburg

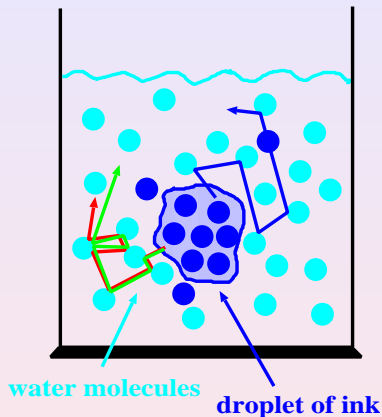
10 March 2011



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?

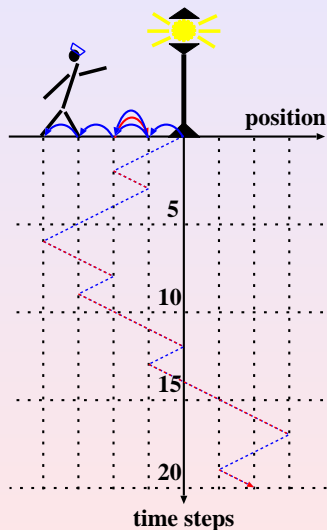


- dispersion of a droplet of ink by *diffusion*
- assumption: *chaotic collisions* between billiard balls

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:

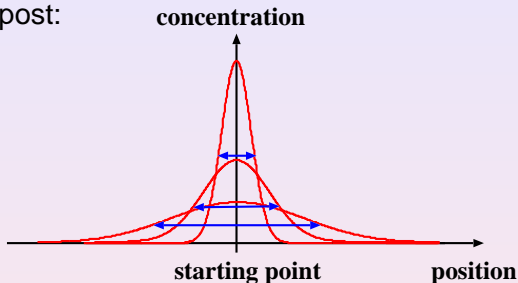
random walk in one dimension:

- 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 ρ at time step n

A. Einstein (1905)

Basic idea of deterministic chaos

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

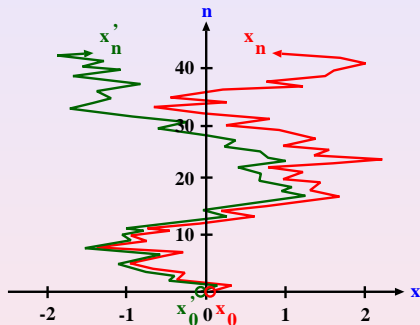
simple equation of motion

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

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

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

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



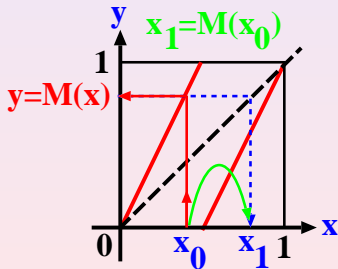
- the starting point **determines** where the sailor will move
- **sensitive dependence** on initial conditions

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:

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

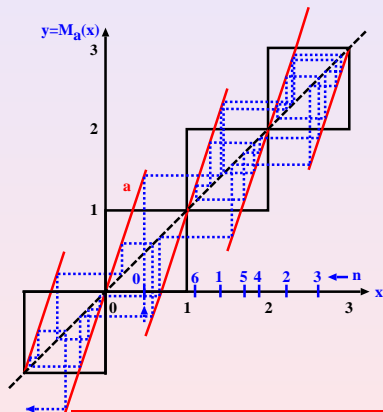
$\lambda := \ln 2$: **Ljapunov exponent**; A.M.Ljapunov (1892)

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

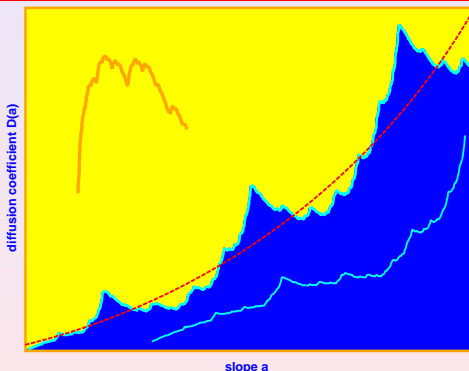
structure of formula:

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

Parameter-dependent deterministic diffusion

exact analytical results for this model:

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

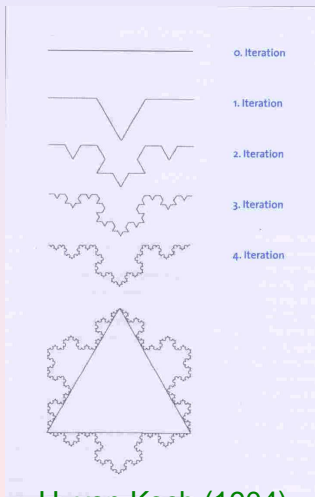


compare diffusion of drunken sailor with chaotic model:

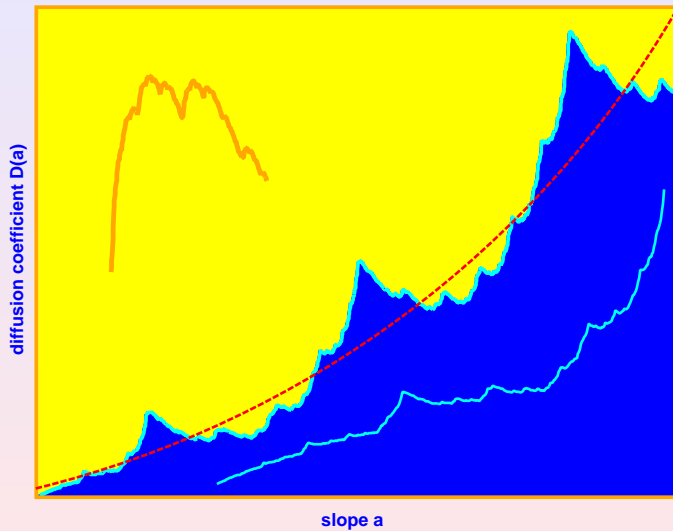
⊃ **fine structure beyond simple random walk solution**

R.K., Dorfman, PRL (1995)

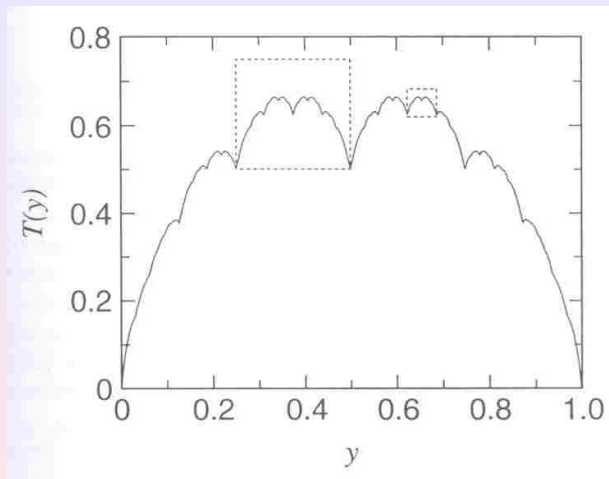
Fractals 1: von Koch's snowflake



H. von Koch (1904)

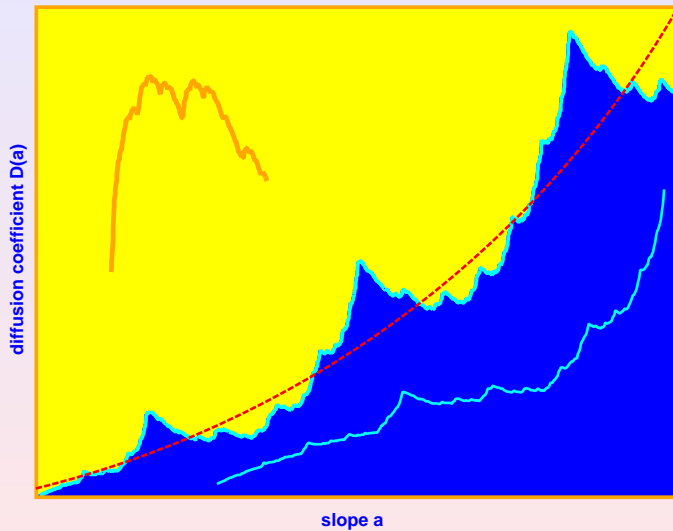


Fractals 2: the Takagi function

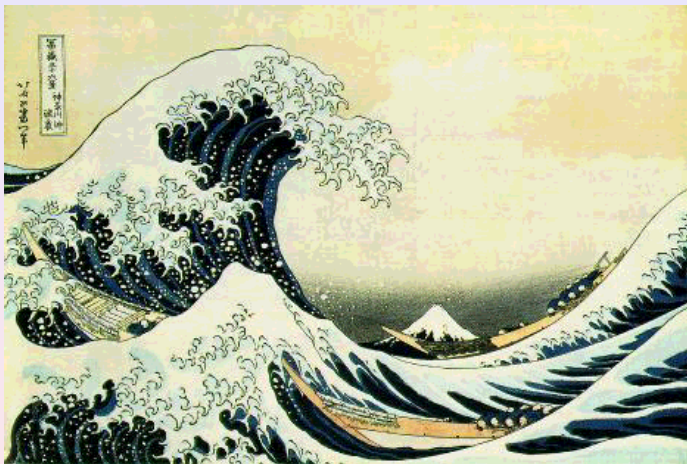


T.Takagi (1903)

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



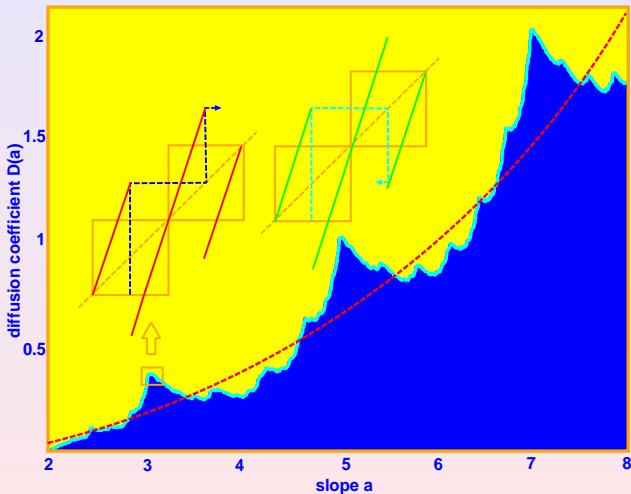
'Fractals 3': art meets science



K.Hokusai (1760-1849)

The great wave of Kanagawa; woodcut

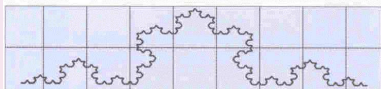
Physical explanation of the fractal structure



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 ϵ
- **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)

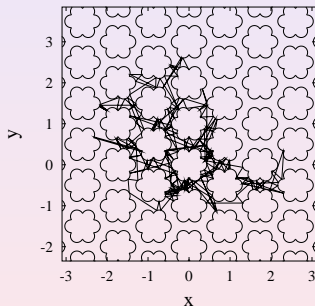
The flower-shaped billiard

deterministic diffusion in physically more realistic models:

Hamiltonian particle billiards

example:

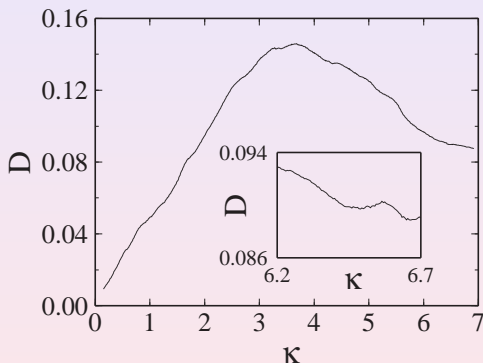
flower-shaped hard disks on a two-dimensional periodic lattice
moving **point particles** collide elastically with the disks *only*:
Knudsen diffusion (1909)



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:



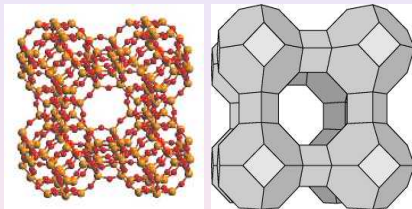
again a non-monotonic function of the control parameter with **irregular structure on fine scales**

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

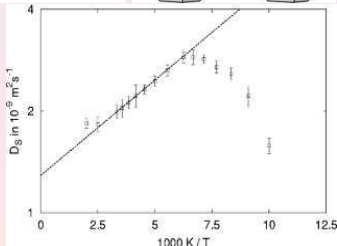
example: unit cell of **Linde type A zeolite**; strictly periodic structure built by a “cage” of silica and oxygen



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, antidot lattices, Josephson junctions, vibratory conveyors (see tomorrow); optical lattices?**

Acknowledgements and literature

work performed with:

J.R.Dorfman (College Park, USA), P.Gaspard (Brussels),
T.Harayama (Kyoto)

literature:

