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

School of Mathematical Sciences, Queen Mary University of London
Institute of Theoretical Physics, Technical University of Berlin
London Mathematical Laboratory

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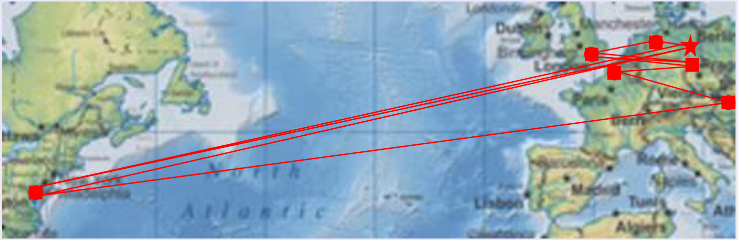
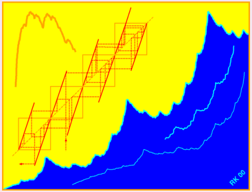
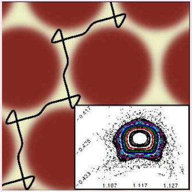
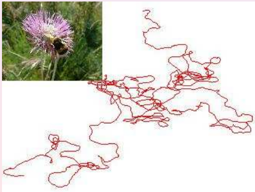
Diffusive dynamics



my scientific trajectory; and my research themes:





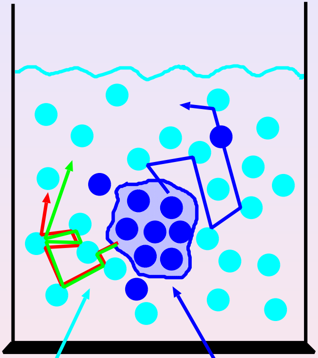


chaos, complexity and nonequilibrium statistical physics with applications to nanosystems and biology

Outline of this talk

1. **Motivation:** microscopic chaos, random walks and diffusion
2. A simple model for **chaotic diffusion**...
3. ...yields a **fractal diffusion coefficient**
4. From simple models towards experiments: **small systems**

Microscopic chaos in a glass of water?



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

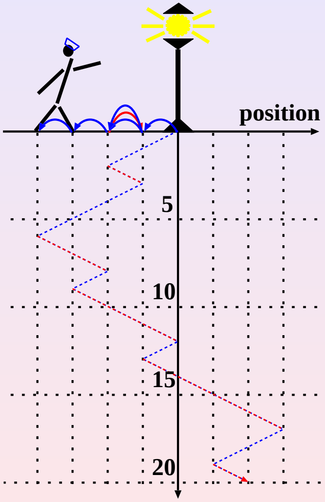
microscopic chaos
⇓
macroscopic diffusion

Gallavotti, Cohen (1995)

from *stochastic* Brownian motion to *deterministic* chaos:

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*

K. Pearson (1905)

- diffusion coefficient:

$$D = \lim_{n\to\infty} \frac{1}{2n} < [x(n) - x(0)]^2 >$$

$< \ldots >$ *ensemble average*

A. Einstein (1905)

for *sailor:* $D = s^2/2$

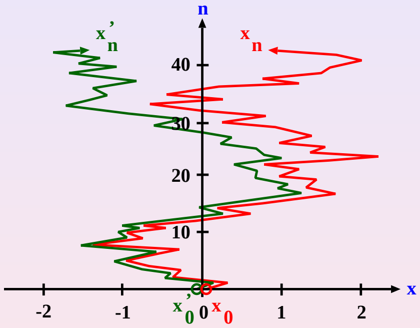
Basic idea of deterministic chaos

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

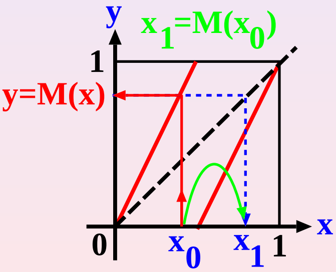
E.N. Lorenz (1963)

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:

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

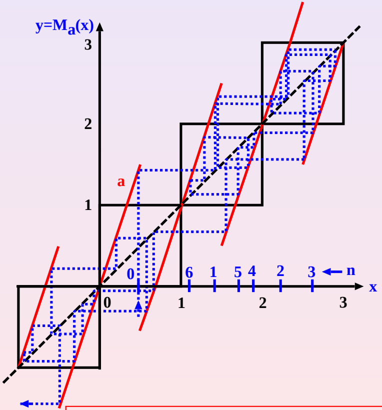
$\lambda := \ln 2$: **Ljapunov exponent**; A.M.Ljapunov (1892)

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

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

Taylor-Green-Kubo formula

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

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

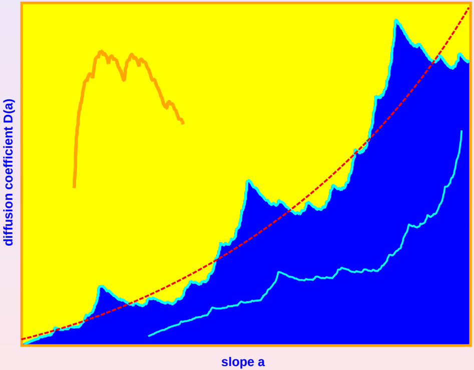
2. intra-cell dynamics: $\varrho_a(x)$ is obtained from the Liouville equation of the map on the unit interval

structure of formula:
first term yields **random walk**, others higher-order **correlations**

Parameter-dependent deterministic diffusion

exact analytical result for this model:

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

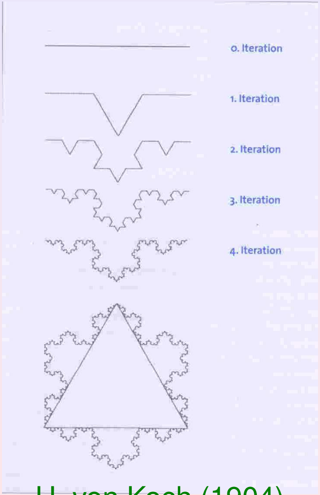


compare diffusion of drunken sailor with chaotic model:

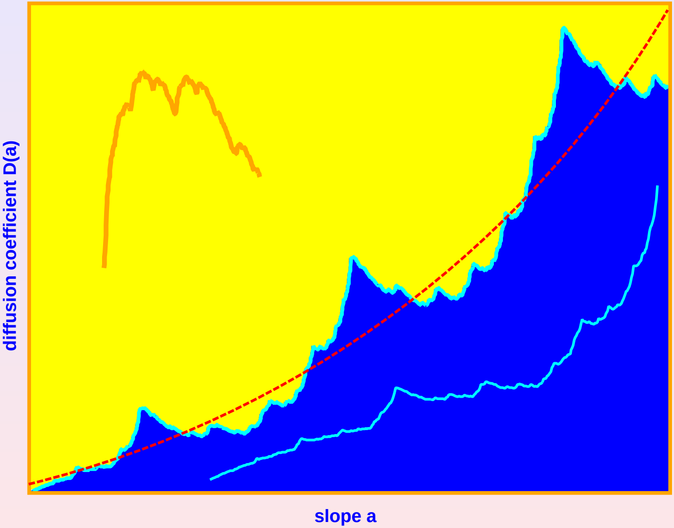
$\exists$ **fine structure beyond simple random walk solution**

RK, Dorfman, PRL (1995)

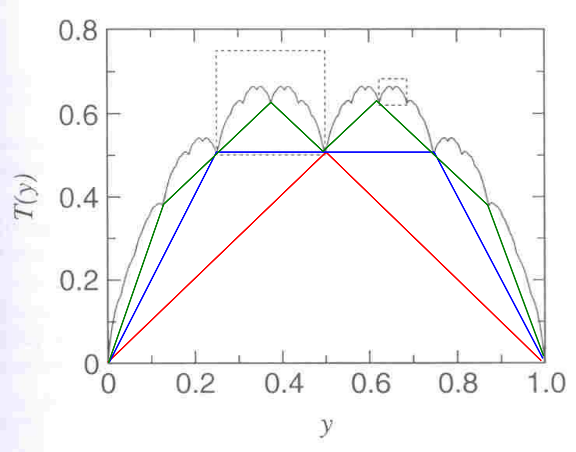
Fractals 1: von Koch's snowflake



H. von Koch (1904)

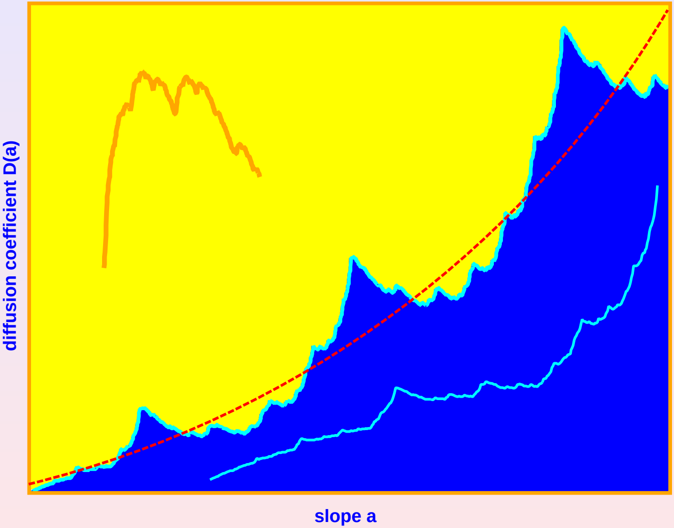

diffusion coefficient D(a)
slope a

Fractals 2: the Takagi function

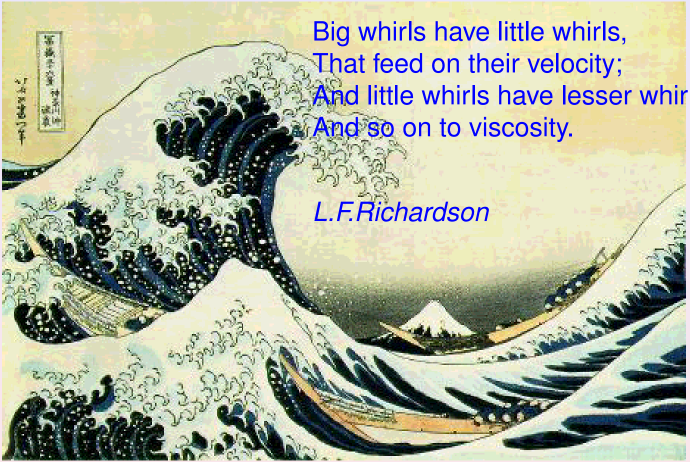


T.Takagi (1903)

example of a continuous but nowhere differentiable function

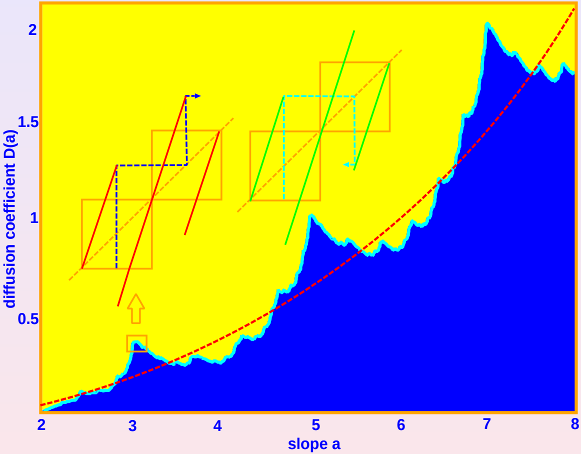

diffusion coefficient D(a)
slope a

‘Fractals 3’: art meets science



K.Hokusai (1760-1849)
The great wave of Kanagawa; woodcut

Physical explanation of the fractal structure

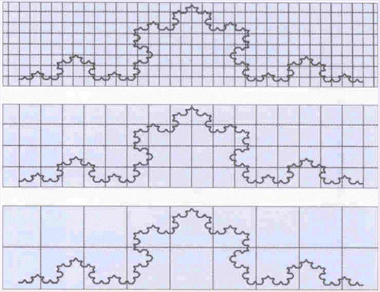


memory: local extrema due to sequences of (higher order) **correlated microscopic scattering processes**

$\exists$ exact formula D(chaos quantities) (Gaspard, Nicolis, 1990)

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: $N \sim \epsilon^{-\mathbf{d}}$

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

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

$$N(\epsilon) = C_1 \epsilon^{-1} (1 + C_2 \ln \epsilon)^{\alpha}$$

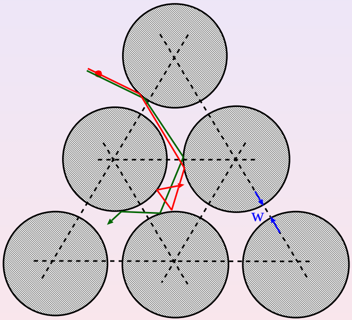
with $0 \leq \alpha \leq 1.2$ locally varying

Keller, Howard, RK (2008)

The periodic Lorentz gas

deterministic diffusion in physically more realistic models:

Small Systems; e.g., Bustamante, Liphardt, Ritort (2005)



Lorentz (1905)

point particle scatters elastically with *hard disks* on a *triangular lattice*

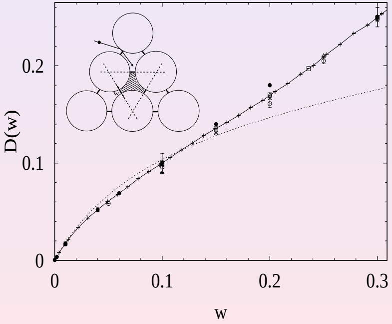
only nontrivial control parameter: gap size w, cf. density of scatterers

paradigmatic example of a **chaotic** Hamiltonian particle billiard:
∃ positive Ljapunov exponent;
∃ diffusion in certain range of w
Bunimovich, Sinai (1980)

Question: How does the diffusion coefficient $D(w)$ look like?

Diffusion coefficient for the periodic Lorentz gas

diffusion coefficient $D(w) = \lim_{t\to\infty} < (\mathbf{r}(t) - \mathbf{r}(0))^2 > /(4t)$
computer simulation results:



- dots: random walk approx. by Machta, Zwanzig (1983)

Diffusion coefficient for the periodic Lorentz gas

diffusion coefficient $D(w) = \lim_{t\to\infty} < (\mathbf{x}(t) - \mathbf{x}(0))^2 > /(4t)$

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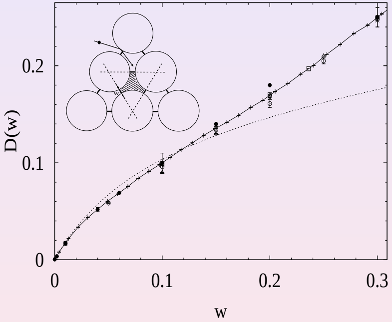
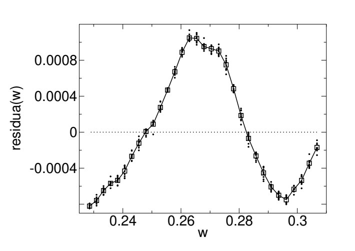


residua for large w:

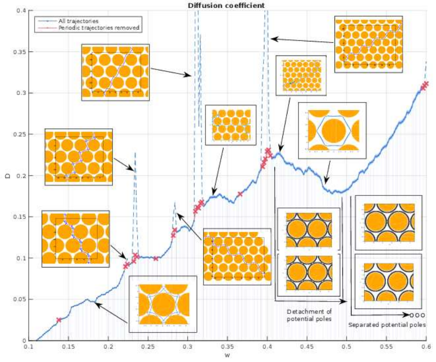


- dots (left): random walk approx. by Machta, Zwanzig (1983)
- $\exists$ irregularities on fine scales; RK, Dellago (2000)

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

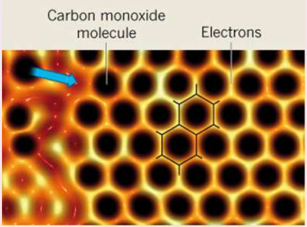
From diffusion in soft potentials to artificial graphene

replace hard scatterers by soft repulsive (Fermi) potentials;
simulation results for diffusion coefficient $D(w)$ of a point particle as a function of gap size w (Gallegos et al., PRL, 2019):



superdiffusive singularities with $\langle x^2 \rangle \sim n^\alpha$, $\alpha > 1$ by periodic orbits

may model diffusion of electrons in CO molecules on CU(1,1,1) surface:



Gomes et al., Nature (2012)

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 spatially periodic *small* systems

- **open question:** clearcut verification in experiments? good candidates: nanopores, antidot lattices, Josephson junctions, vibratory conveyors, graphene? optical lattices?

Acknowledgements and literature

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