Deterministic chaos and diffusion in maps and billiards

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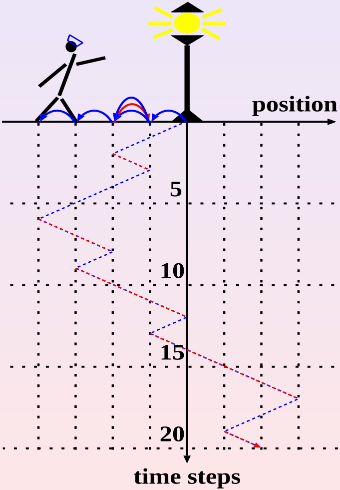
Mathematics for the Fluid Earth
Newton Institute, Cambridge, 14 November 2013

Outline

1. **diffusion in simple chaotic maps**
   - motivation: from stochastic to deterministic random walks
   - simple maps with non-trivial diffusion coefficients
2. **diffusion in chaotic particle billiards**
   - density-dependent diffusion in the periodic Lorentz gas
   - from theory towards applications

The drunken sailor at a lamppost

random walk in one dimension (K. Pearson, 1905):



- steps of length s with probability $p(\pm s) = 1/2$ to the left/right
- single steps *uncorrelated*: Markov process
- define diffusion coefficient as

$$D := \lim_{n\to\infty} \frac{1}{2n} < (x_n - x_0)^2 >$$

with discrete time step $n \in \mathbb{N}$ and average over the initial density $< \ldots > := \int dx \;\varrho(x) \ldots$ of positions $x = x_0 \;,\; x \in \mathbb{R}$

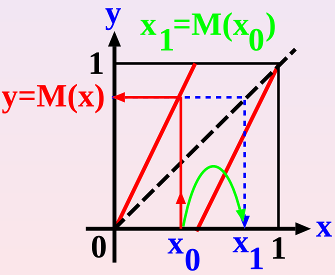
- for *sailor:* $D = s^2/2$

Dynamics of a chaotic map

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

key idea: use chaos instead of stochasticity for drunken sailor
why? determinism preserves all dynamical correlations

model a single step $x_0 \to x_1$ by a *deterministic map*:



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

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

with

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

Bernoulli shift

Lyapunov exponent: $\lambda = \ln 2 > 0$
paradigm of a *chaotic map*

A deterministic random walk

2. study diffusion in the piecewise linear deterministic map

$$M_h(x) = \begin{cases} 2x + h & 0 \le x < \frac{1}{2} \\ 2x - 1 - h & \frac{1}{2} \le x < 1 \end{cases}$$

lifted onto the real line by

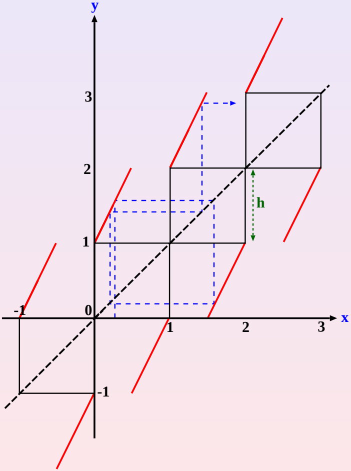
$$M_h(x+1) = M_h(x) + 1$$

with symmetric shift $h \ge 0$ as a control parameter (Gaspard, RK, 1998)

deterministic random walk generated by

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

problem: calculate $D(h)$



Geisel/Grossmann/Kapral (1982)

The Takagi function method

start from the Einstein formula

$$D = \lim_{n\to\infty} \frac{1}{2n} < (x_n - x_0)^2 > \, , \; x = x_0 \; ,$$

with $< \ldots >= \int_0^1 dx \; \varrho_h(x) \ldots$ over the invariant density $\varrho_h(x)$ of $m_h(x) := M_h(x)$ mod 1; it is $\forall_h \; \varrho_h(x) = 1$!
define *integer jumps* $j_k = \lfloor x_{k+1} \rfloor - \lfloor x_k \rfloor$ at discrete time k and rewrite $D(h)$ via telescopic summation to

$$D(h) = \frac{1}{2}\left\langle j_0^2 \right\rangle + \sum_{k=1}^{\infty} \langle j_0 j_k \rangle$$

Taylor-Green-Kubo formula

structure of formula:
first term: random walk solution
other terms: higher-order dynamical correlations

Generalized Takagi/de Rham functions

problem: calculate $\langle j_0 \sum_{k=0}^{\infty} j_k \rangle = \int_0^1 dx\, j_0 \sum_{k=0}^{\infty} j_k$

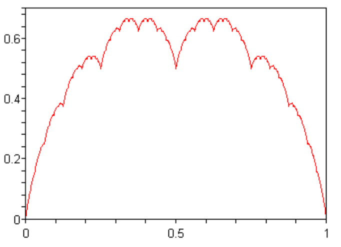
defining $T_h^n(x) = \int_0^x dy \sum_{k=0}^{n} j_k(y)$ yields the de Rham-type equation

$$T_h^n(x) = t(x) + \frac{1}{2} T_h^{n-1}(m_h(x))$$

with $dt(x)/dx := j_0(x)$.

example: for $h = 1$ we get the famous Takagi function (1903)

$$T_1^n(x) = \begin{cases} x + \frac{1}{2} T_1^{n-1}(2x) & 0 \le x < \frac{1}{2} \\ 1 - x + \frac{1}{2} T_1^{n-1}(2x-1) & \frac{1}{2} \le x < 1 \end{cases}$$



Solving the functional recursion relation

$$T_h^n(x) = t(x) + \frac{1}{2}\, T_h^{n-1}(m_h(x))$$

can be solved to

$$T_h^n(x) = \sum_{k=0}^{n} \frac{1}{2^k} t(m_h^k(x))$$

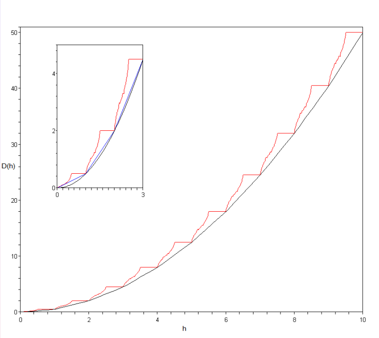
For $0 \leq h$ and $T_h(x) = \lim_{n\to\infty} T_h^n(x)$ this leads to

$$D(h) = \frac{\lceil h \rceil^2}{2} + \left(\frac{1-\hat{h}}{2}\right)(1 - 2\lceil h \rceil) + T_h\left(\hat{h}\right)$$

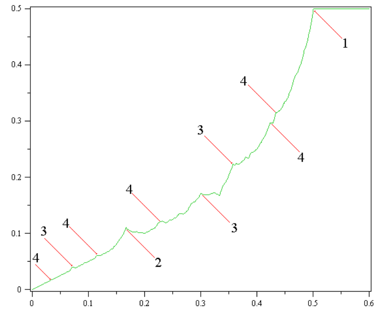
Knight, RK, Nonlinearity (2011)

(with $\hat{h} := h \mod 1\ (h \notin \mathbb{N}), \hat{h} := 1\ (h \in \mathbb{N}), \hat{h} := 0\ (h = 0)$)

Diffusion coefficient for the lifted Bernoulli shift



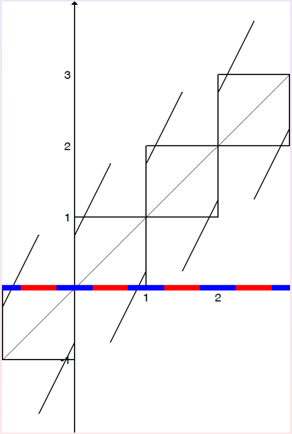
On large scales we recover the drunken sailor's result, $D(h) \sim h^2/2 \; (h \gg 1)$.



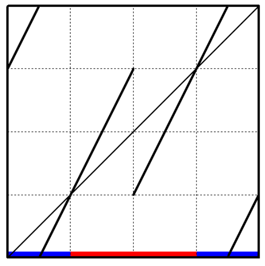
On small scales, $D(h)$ is *partially* a fractal function. Local maxima are the solutions to $m_h^n(1/2) = 1/2$: **topological instability** under parameter variation.

Why the plateau regions?

For $0.5 \leq h \leq 1$ ergodicity is broken and topology conserved:



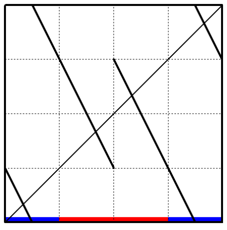
The phase space is split up into two invariant sets, see the mod 1 map:



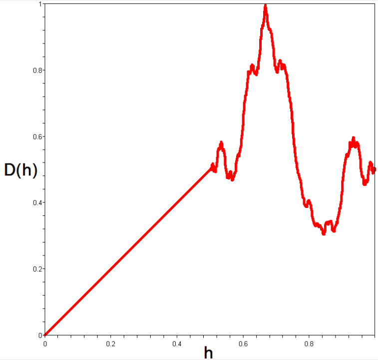
For a *uniform initial density*, the diffusion coefficient is calculated to $D(h) = D(h) + D(h) = (1 - h) + (h - \frac{1}{2}) = \frac{1}{2}$.

More maps: the lifted negative Bernoulli shift

Same Takagi function method:



$0 \leq h \leq 0.5$: again ergodicity breaking

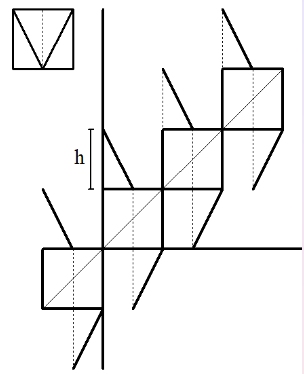


$0.5 \leq h \leq 1$: topological instability

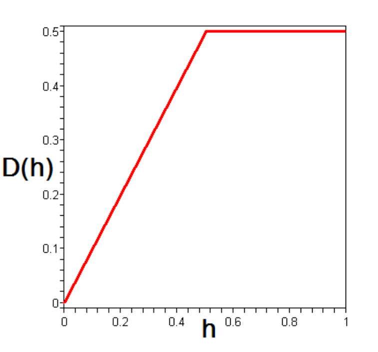
which suggests:

topological instability $\Leftrightarrow$ fractal diffusion coefficient
non-ergodicity $\Leftrightarrow$ linear diffusion coefficient

The lifted V-map



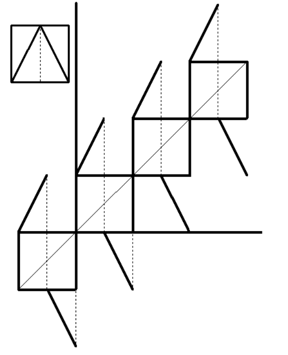
This map suggests topological instability under parameter variation and no ergodicity breaking...



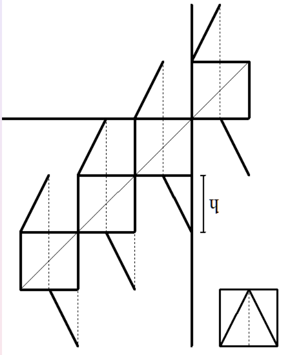
...but Takagi function method yields a piecewise linear $D(h)$: explanation via *dominating branch*

The lifted tent map

Finally, the lifted tent map $T(x)$...



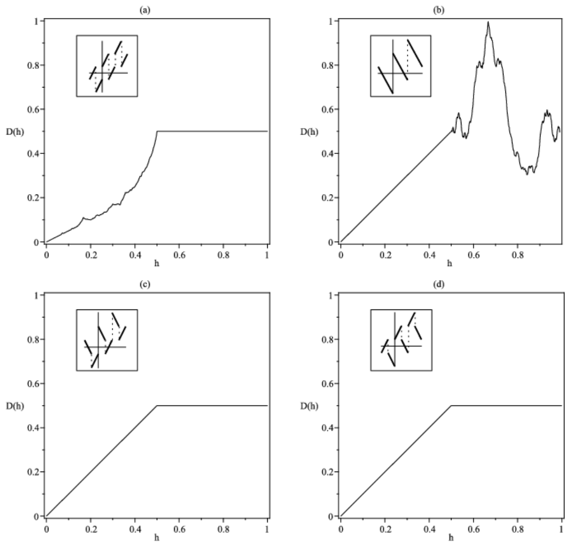
...via $T(x) = -V(-x)$:



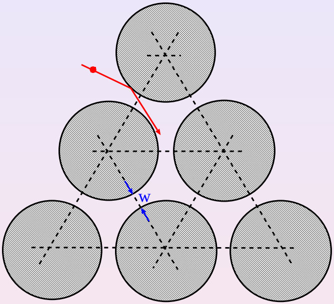
...is topologically conjugate to the V-map $V(x)$...

Fortunately, $D(h)$ is invariant under topological conjugacy (Korabel, RK, 2004): $\nexists$ Takagi function solution for this map!

Summary: Linear and fractal diffusion coefficients



The periodic Lorentz gas

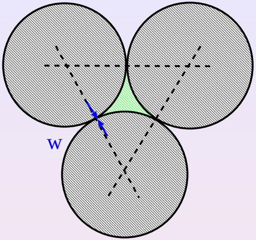


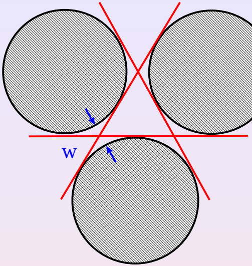
Lorentz (1905)

moving point particle of unit mass with unit velocity scatters elastically with hard disks of unit radius on a triangular lattice

only nontrivial control parameter: gap size w

two limiting cases for diffusion under parameter variation:





$w_0 = 0$, $D(w_0) = 0$ $w_\infty \simeq 0.3094$, $D(w_\infty) \to \infty$

trivial localization ballistic flights

paradigmatic example of a **chaotic** Hamiltonian particle billiard:

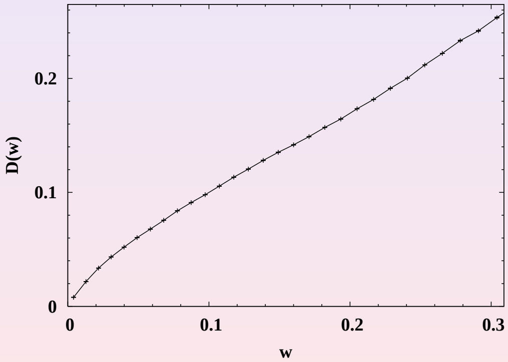
$\exists$ positive Ljapunov exponent; $\exists D(w)$, $w_0 < w < w_\infty$

Bunimovich, Sinai (1980)

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

Diffusion coefficient for the periodic Lorentz gas

diffusion coefficient $D(w) = \lim_{t\to\infty} \frac{<(\mathbf{x}(t)-\mathbf{x}(0))^2>}{4t}$ from MD simulations (RK, Dellago, 2000):



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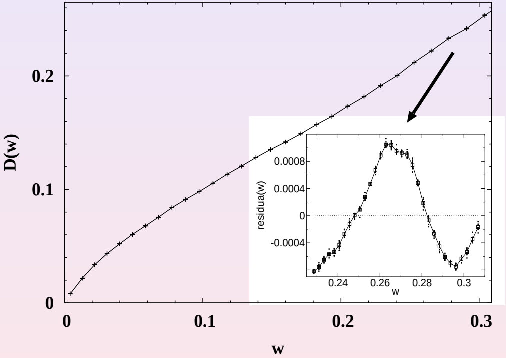
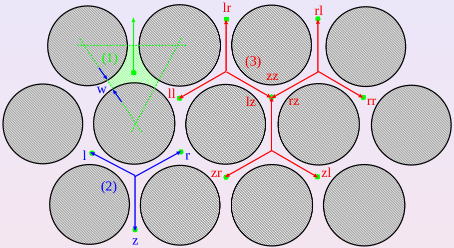


$\exists$ irregularities on fine scales

Can one understand these results on an analytical basis?

Taylor-Green-Kubo formula for billiards

map diffusion onto *correlated random walk* on hexagonal lattice:



rewrite diffusion coefficient as Taylor-Green-Kubo formula:

$$D(w) = \frac{1}{4\tau}\left\langle \mathbf{j}^2(\mathbf{x}_0)\right\rangle + \frac{1}{2\tau}\sum_{n=1}^{\infty}\langle \mathbf{j}(\mathbf{x}_0)\cdot\mathbf{j}(\mathbf{x}_n)\rangle$$

τ: rate for a particle leaving a trap; $\mathbf{j}(\mathbf{x}_n)$: *inter-cell* jumps over distance ℓ at the nth time step τ in terms of lattice vectors $\ell_{\alpha\beta\gamma\ldots}$

RK, Korabel (2002)

TGK formula can be evaluated to

$$D_n(w) = \frac{\ell^2}{4\tau} + \frac{1}{2\tau} \sum_{\alpha\beta\gamma\ldots}^{n} p(\alpha\beta\gamma\ldots)\boldsymbol{\ell} \cdot \boldsymbol{\ell}(\alpha\beta\gamma\ldots)$$

$p(\alpha\beta\gamma\ldots)$: probability for lattice jumps with this symbol sequence

first term: random walk solution for diffusion on a two-dimensional lattice, calculated to (Machta, Zwanzig, 1983)

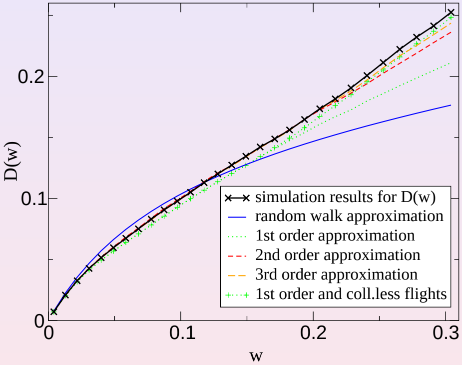
$$D_0(w) = \frac{w(2+w)^2}{\pi[\sqrt{3}(2+w)^2 - 2\pi]}$$

other terms: higher-order dynamical correlations;

for time step 2τ: $D_1(w) = D_0(w) + D_0(w)\,[1 - 3p(z)]$

3τ: $D_2(w) = D_1(w) + D_0(w)\,[2p(zz) + 4p(lr) - 2p(ll) - 4p(lz)]$

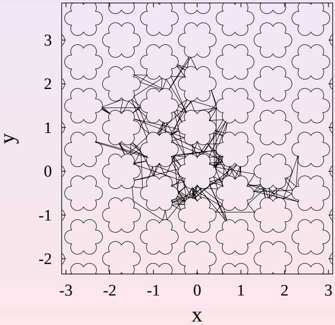
open problem: conditional probabilities $p(\alpha\beta\gamma\dots)$ analytically?
here results obtained from simulations:



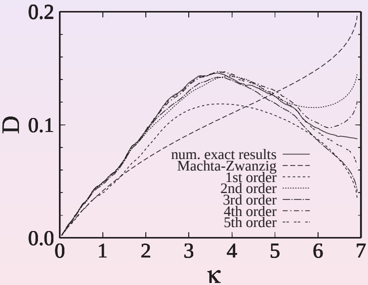
$\Rightarrow$ variation of convergence as a function of w indicates presence of **memory** due to dynamical correlations

Diffusion in the flower-shaped billiard

hard disks replaced by flower-shaped scatterers with petals of curvature κ:



simulation results for the diffusion coefficient and analysis as before:



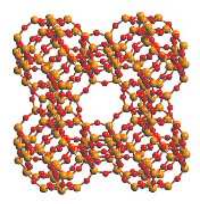
Harayama, RK, Gaspard (2002)

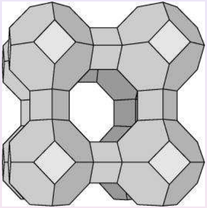
$\Rightarrow \exists$ irregular diffusion coefficient due to dynamical correlations

Outlook: molecular diffusion in zeolites

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

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

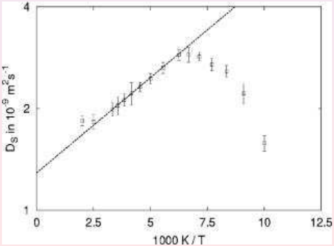




Schüring et al. (2002): MD simulations with ethane yield non-monotonic temperature dependence of *diffusion coefficient*

$$D(T) = \lim_{t\to\infty} \frac{<[\mathbf{x}(t) - \mathbf{x}(0)]^2>}{6t}$$

in Arrhenius plot; explanation similar to previous TGK expansion



Summary

- $\exists$ **fractal transport coefficients in simple maps**
- $\exists$ **irregular transport coefficients** of the same origin in **particle billiards**

I expect this phenomenon to be **typical** for *classical* transport in *low-dimensional, deterministic, spatially periodic chaotic* systems.

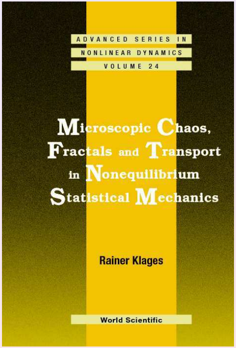
'Advertisement'

- **similar results for:**
  - current and diffusion in the piecewise linear map $M_{a,b}(x) = ax + b\ ,\ x \in [0, 1)$
  - diffusion in the climbing sine map $C_a(x) = x + k\sin(2\pi x)$
  - diffusion in a dissipative particle billiard with oscillatory driving
- **furthermore:**
  - fractal parameter dependencies for mobility, chemical reaction rate, anomalous diffusion in simple maps
  - stability of such curves with respect to random perturbations
  - some indication of such phenomena in experiments: *antidot lattices, granular vibratory conveyors, surface diffusion, Josephson junctions,* **zeolites**

Acknowledgements and literature

work performed in collaboration with:

G.Knight (Bologna)
Chr.Dellago (Vienna)
J.R.Dorfman (College Park/USA)
P.Gaspard (Brussels)
T.Harayama (Kyoto)
N.Korabel (Manchester)



Part 1