The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization
IAEA
International Atomic Energy Agency

2058-S-1

Pseudochaos and Stable-Chaos in Statistical Mechanics and Quantum Physics

21 - 25 September 2009

From normal to anomalous deterministic diffusion (I): Normal deterministic diffusion

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From normal to anomalous deterministic diffusion
Part 1: Normal deterministic diffusion

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ICTP, 21 September 2009

General setup

nonequilibrium conditions →

		equilibrium	nonequilibrium steady states	nonequilibrium non-steady states
microscopic	dynamical systems	ergodic hypothesis	**microscopic chaos** strong	weak
↓	statistical mechanics	Gibbs ensembles	**complexity** fractal SRB measures	infinite measures
macroscopic	thermodynamics	thermodynamic properties	**deterministic transport** normal	anomalous

⇨ general theory of nonequilibrium statistical physics starting from microscopic chaos?

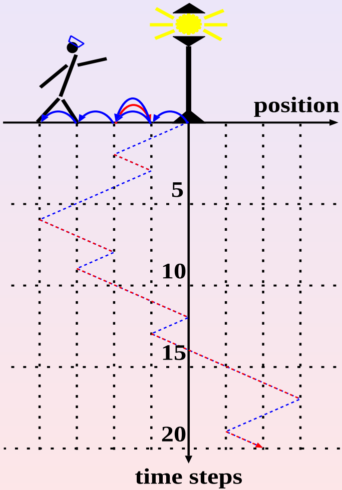
Outline

two parts:

1. **Normal deterministic diffusion:**
   simple maps and billiards, dynamical systems theory, and zeolites
2. **Anomalous deterministic diffusion:**
   some slightly more complicated maps, ergodic and stochastic theory, and cell migration

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

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

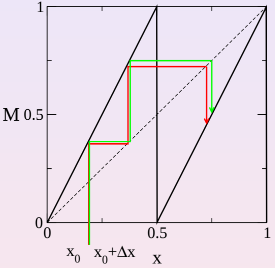
with discrete time step $n \in \mathbb{N}$ and average over the initial density $< \ldots > := \int dx \ \varrho(x) \ldots$ of positions $x = x_0 \ , \ x \in \mathbb{R}$

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

Bernoulli shift and dynamical instability

idea: generate single steps from deterministic chaos

Bernoulli shift $M(x) = 2x \mod 1$ with $x_{n+1} = M(x_n)$:



apply small perturbation $\Delta x_0 := \tilde{x}_0 - x_0 \ll 1$ and iterate:

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

$\Rightarrow$ **exponential** dynamical instability with **Ljapunov exponent**

$$\lambda := \ln 2$$

Ljapunov exponent

definition for one-dimensional maps via *time average*:

$$\lambda(x) := \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} \ln |M'(x_i)| \; , \; x = x_0$$

if map is ergodic: time average = ensemble average,

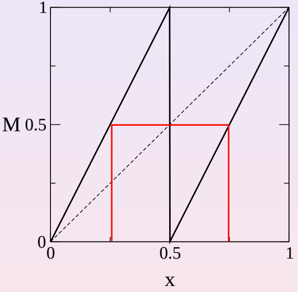
$$\lambda = \langle \ln |M'(x)| \rangle \quad \textbf{Birkhoff's theorem}$$

with average over an invariant probability density $\varrho(x)$ that is related to the map's SRB measure via $\mu(x) = \int_0^x dy\, \varrho(y)$

Bernoulli shift is *expanding*: $\forall x \, |M'(x)| > 1$, hence 'hyperbolic'

normalizable pdf exists, here simply $\varrho(x) = 1 \Rightarrow \lambda = \ln 2$

Kolmogorov-Sinai entropy



- define a partition $\{W_i^n\}$ of the phase space and *refine* it by iterating the critical point n times backwards
- let $\mu(w)$ be the SRB measure of a partition element $w \in \{W_i^n\}$
- define $H_n := -\sum_{w \in \{W_i^n\}} \mu(w) \ln \mu(w)$,

  where n denotes the level of refinement
- the limit $h_{ks} := \lim_{n\to\infty} \frac{1}{n} H_n$

  defines the Kolmogorov-Sinai (metric) entropy (if the partition is generating)

for Bernoulli shift with uniform measure refinement yields $H_n = n \ln 2$, hence $h_{ks} = \ln 2$

Pesin theorem

note: for Bernoulli shift $\lambda = \ln 2$ and $h_{ks} = \ln 2$

Theorem

For closed C^2 Anosov systems the KS-entropy is equal to the sum of positive Lyapunov exponents.
Pesin (1976), Ledrappier, Young (1984)

believed to hold for a wider class of systems

for one-dimensional hyperbolic maps: $\boxed{h_{ks} = \lambda}$

A deterministic random walk

study diffusion in the piecewise linear deterministic map

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

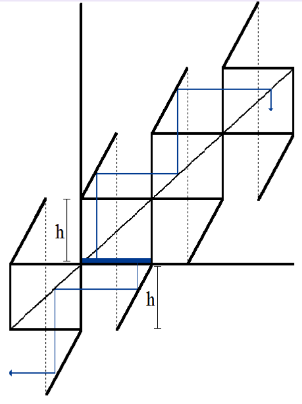
lifted onto the real line by

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

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

deterministic random walk generated by

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



Geisel/Grossmann/Kapral (1982)

Calculating deterministic diffusion coefficients

problem: What is the deterministic diffusion coefficient $D(h)$?

1. $\exists$ many different methods for calculating $D(h)$
   $\rightarrow$ Artuso, Cristadoro
2. the *escape rate approach* enables to express the diffusion coefficient in terms of dynamical systems quantities:

$$D(h) = \lim_{L\to\infty} \left(\frac{L}{\pi}\right)^2 [\lambda(\mathcal{R}(h)) - h_{KS}(\mathcal{R}(h))] ,$$

Gaspard, Nicolis, Dorfman (1990ff)

where L is the chainlength of the map and $\mathcal{R}(h)$ the fractal repeller under absorbing boundary conditions

The Takagi function method

start from

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

with $< \ldots > := \int_0^1 dx \; \varrho_h(x) \ldots$ over the invariant density 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: leads to 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 $dt(x)/dx := j_0(x)$; can be solved to

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

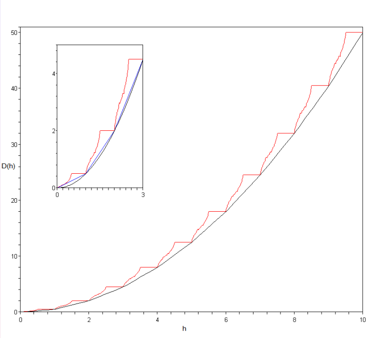
For $0 \leq h$ and $T_h(x) := \lim_{n\to\infty} T_h^n(x)$ this leads to

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

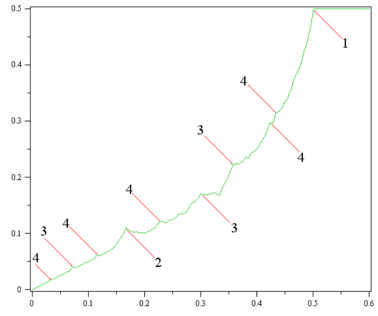
(Knight, R.K., 2008)

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, $D(h) \sim h^2/2 \; (h \gg 1)$

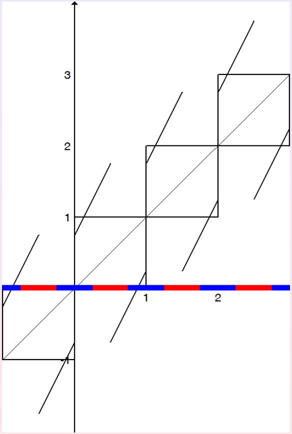


on small scales, $D(h)$ is *partially* a fractal function

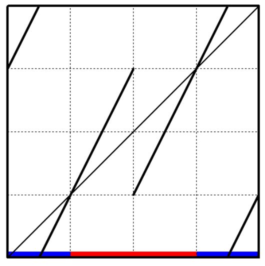
Local maxima are the solutions to $m_h^n(1/2) = 1/2$: **topological instability** under parameter variation.

Why the plateau regions?

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



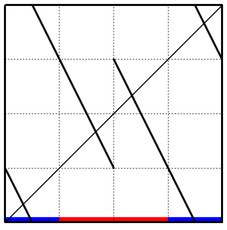
The phase space is split up into two invariant sets, see the $\mod 1$ map:



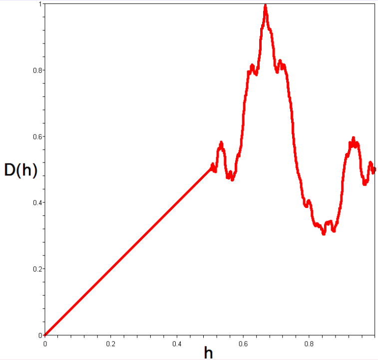
For a *uniform initial density*, the diffusion coefficient is calculated to $D(h) = D(h) + D(h) = (1 - h) + (h - \frac{1}{2}) = \frac{1}{2}$.

More maps: the lifted negative Bernoulli shift

Same Takagi function method:



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

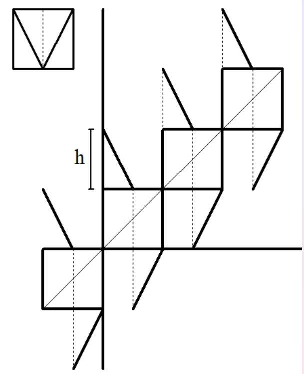


$0.5 \le h \le 1$: topological instability

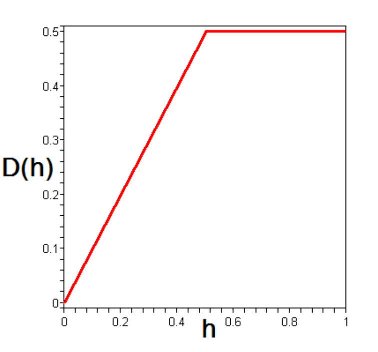
which suggests:

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

The lifted V-map



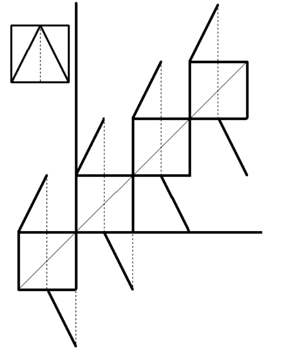
This map suggests topological instability under parameter variation and no ergodicity breaking...



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

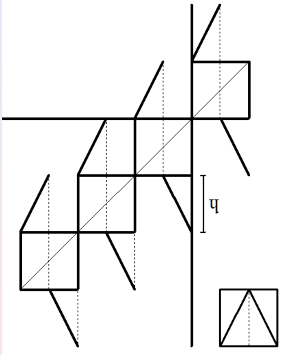
The lifted tent map

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



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

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



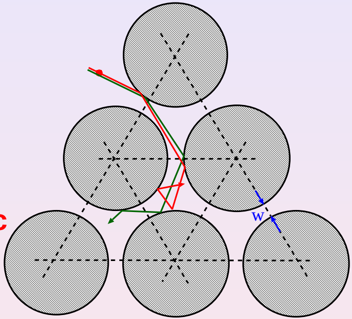
Fortunately, $D(h)$ is invariant under topological conjugacy (Korabel, R.K., 2004): ∄ Takagi function solution for this map!

The periodic Lorentz gas

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

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

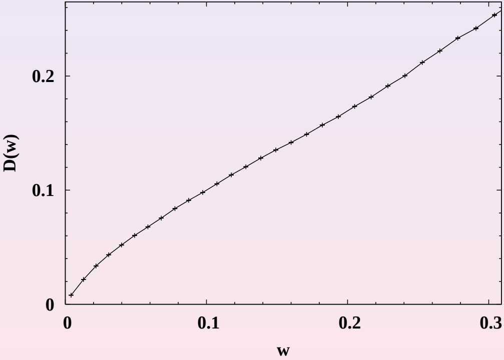


Lorentz (1905)

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 (R.K., Dellago, 2000):



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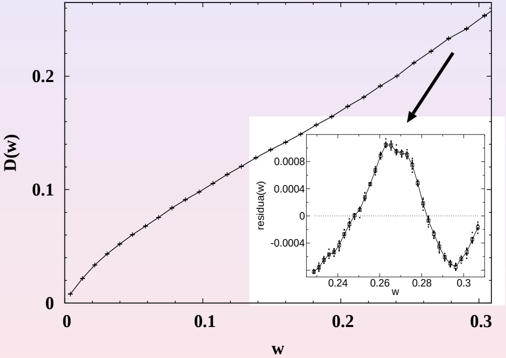
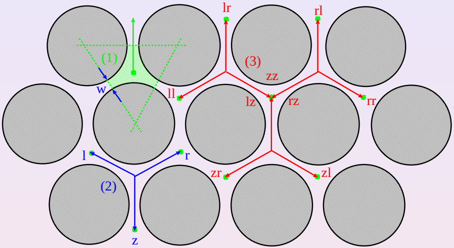


$\exists$ irregularities on fine scales

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 $\ell_{\alpha\beta\gamma\ldots}$

R.K., 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)

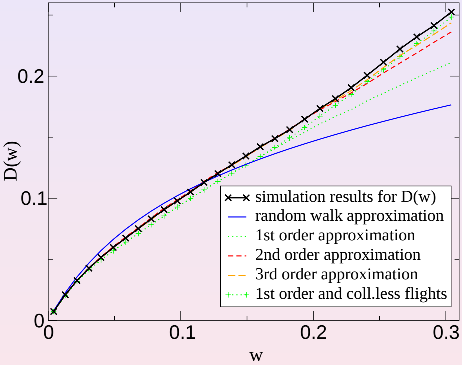
$$D_0(w) = \frac{w(2+w)^2}{\pi[\sqrt{3}(2+w)^2 - 2\pi]}$$

other terms: higher-order dynamical correlations;

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

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

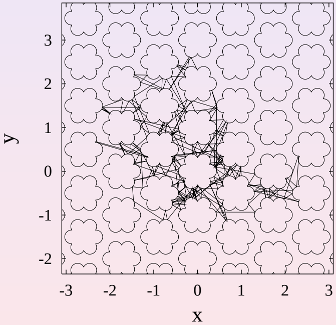
open problem: conditional probabilities $p(\alpha\beta\gamma\ldots)$ analytically?
here results obtained from simulations:



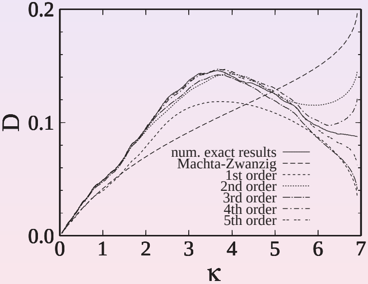
⇒ variation of convergence as a function of w indicates presence of *memory* due to dynamical correlations

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:

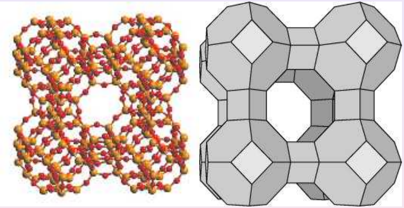


Harayama, R.K., Gaspard (2002)

$\Rightarrow \exists$ *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