From normal to anomalous deterministic diffusion Part 2: From normal to anomalous

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Sperlonga, 20-24 September 2010

Outline

yesterday:

1. **Normal deterministic diffusion:**
   some basics of dynamical systems theory for maps and escape rate theory of deterministic diffusion

reference:

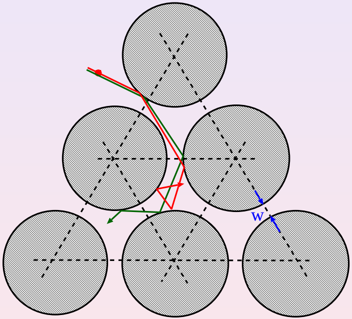
R.Klages,
From Deterministic Chaos to Anomalous Diffusion
book chapter in:
Reviews of Nonlinear Dynamics and Complexity, Vol. 3
H.G.Schuster (Ed.), Wiley-VCH, Weinheim, 2010
http://www.maths.qmul.ac.uk/~klages

today:

2. **From normal to anomalous deterministic diffusion:**
   normal diffusion in particle billiards and anomalous diffusion in intermittent maps

The periodic Lorentz gas

idea: study more physically realistic models of deterministic diffusion



Lorentz (1905)

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

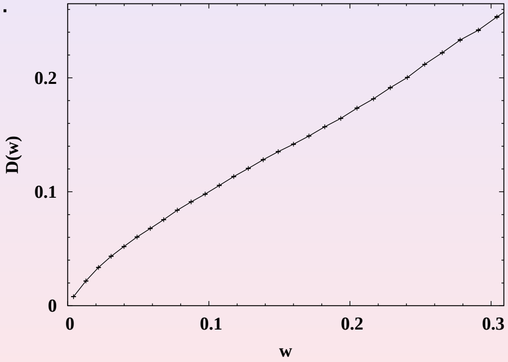
only nontrivial control parameter: gap size w

paradigmatic example of a **chaotic** Hamiltonian particle billiard:
$\exists$ positive Ljapunov exponent;
$\exists$ diffusion in certain range of w
(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:



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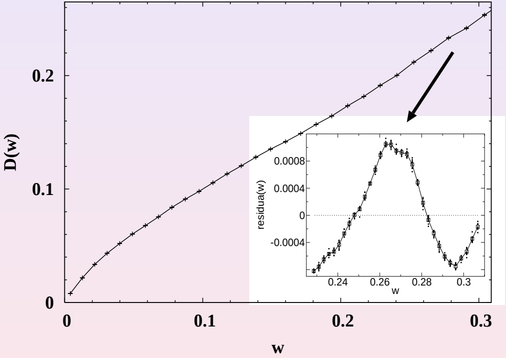
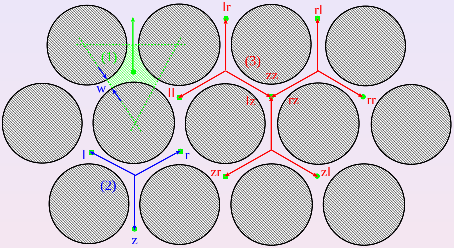


∃ irregularities on fine scales (R.K., Dellago, 2000)

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)

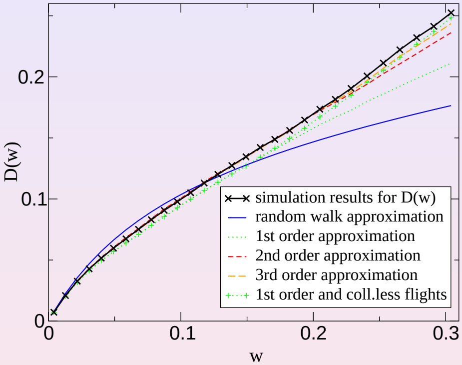
$$D_0(w) = \frac{w(2+w)^2}{\pi[\sqrt{3}(2+w)^2 - 2\pi]}$$

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:

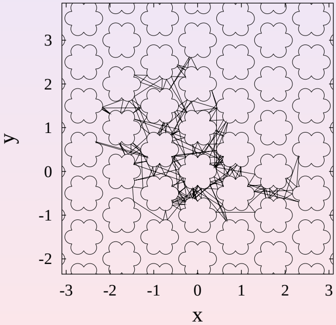


variation of convergence as a function of w indicates presence of **memory** due to dynamical correlations

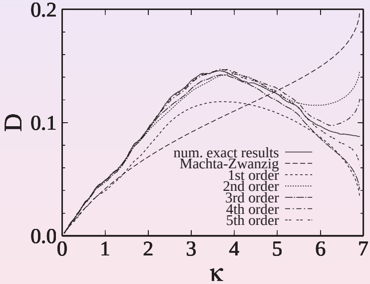
- approach was incorrectly criticized by Gilbert, Sanders (2009)
- theory can be worked out *exactly* for one-dimensional maps

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:



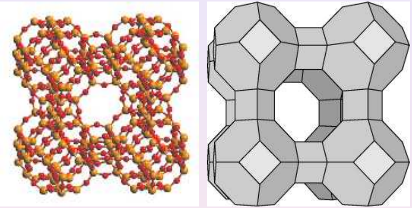
Harayama, R.K., Gaspard (2002)

$\exists$ **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

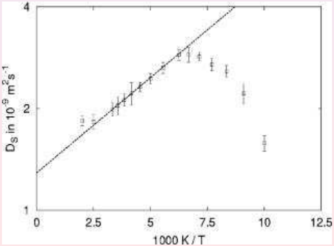
example: unit cell of Linde type A zeolite; periodic structure built by silica and oxygen forming a “cage”



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

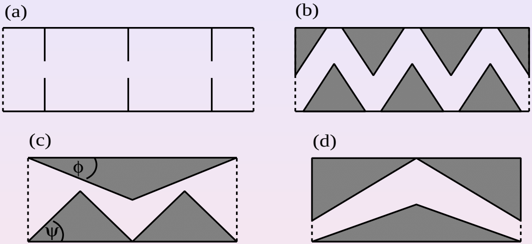
$$D_S(T) = \lim_{t\to\infty} \frac{< [\mathbf{x}(t) - \mathbf{x}(0)]^2 >}{6t}$$

in Arrhenius plot; explanation similar to previous TGK expansion



Polygonal billiard channels

instead of convex scatterers, look at polygonal ones:



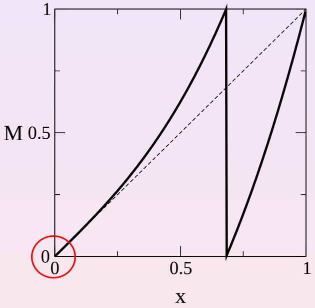
- **weak chaos:** dispersion of nearby trajectories $\Delta(t)$ grows weaker than exponential (Zaslavsky, Usikov, 2001)
- **pseudochaos:** algebraic dispersion $\Delta \sim t^{\nu}$, $0 < \nu$ (Zaslavsky, Edelman, 2002); above: special case $\nu = 1$
- highly non-trivial diffusive and ergodic properties (Artuso, 1997ff; Cecconi, Cencini, Vulpiani, 2000ff; Rondoni, 2006)

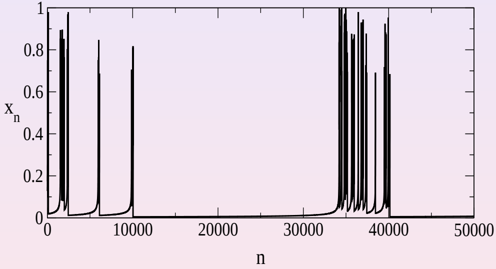
$\exists$ review about pseudochaotic diffusion in book by R.K., 2007

Intermittency in the Pomeau-Manneville map

consider the nonlinear one-dimensional map

$$x_{n+1} = M(x_n) = x_n + a x_n^z \mod 1 \, , \; z \geq 1 \quad , \quad a = 1$$





phenomenology of **intermittency**: long periodic *laminar phases* interrupted by *chaotic bursts*; here due to an indifferent fixed point, $M'(0) = 1$ (Pomeau, Manneville, 1980)

$\Rightarrow$ map not hyperbolic ($\nexists N > 0$ s.t. $\forall x \forall n \geq N \; |(M^n)'(x)| \neq 1$)

Infinite invariant measure and dynamical instability

- **invariant density** of this map calculated to

$$\varrho(x) \sim x^{1-z} \; (x \to 0)$$

Thaler (1983)

is non-normalizable for $z \geq 2$ yielding an **infinite invariant measure**

$$\mu(x) = \int_x^1 dy \, \varrho(y) \to \infty \; (x \to 0)$$

- **dynamical instability** of this map calculated to

$$\Delta x_n \sim \exp\left(n^{\frac{1}{z-1}}\right) \; (z > 2)$$

Gaspard, Wang (1988)

stretched exponential instability yields $\lambda = 0$: defines a second big class of weakly chaotic dynamics (*sporadic*)

From ergodic to infinite ergodic theory

choose a 'nice' *observable* $f(x)$:

- for $1 \le z < 2$ it is $\sum_{i=0}^{n-1} f(x_i) \sim n \ (n \to \infty)$

Birkhoff's theorem: if M is ergodic then $\frac{1}{n}\sum_{i=0}^{n} f(x_i) =< f >_\mu$

- but for $2 \le z$ we have the **Aaronson-Darling-Kac theorem**,

$$\frac{1}{a_n}\sum_{i=0}^{n-1} f(x_i) \xrightarrow{d} \mathcal{M}_\alpha < f >_\mu \ \ (n \to \infty)$$

$\mathcal{M}_\alpha$: random variable with normalized *Mittag-Leffler* pdf

for M it is $a_n \sim n^\alpha$, $\alpha := 1/(z-1)$; integration wrt to Lebesgue measure m suggests

$$\frac{1}{n^\alpha}\sum_{i=0}^{n-1} < f(x_i) >_m \sim < f(x) >_\mu$$

note: for $z < 2$, $\alpha = 1$ $\exists$ absolutely continuous invariant measure μ, and we have an equality; for $z \ge 2$ $\exists$ infinite invariant measure, and it remains a *proportionality*

Defining weak chaos quantities

This motivates to define a **generalized Ljapunov exponent**

$$\Lambda(M) := \lim_{n\to\infty} \frac{\Gamma(1+\alpha)}{n^\alpha} \sum_{i=0}^{n-1} < \ln \left| M'(x_i) \right| >_m$$

and analogously a **generalized KS entropy**

$$h_{KS}(M) := \lim_{n\to\infty} -\frac{\Gamma(1+\alpha)}{n^\alpha} \sum_{w\in\{W_i^n\}} \mu(w) \ln \mu(w)$$

For a piecewise linearization of M one can show analytically

$$h_{KS}(M) = \Lambda(M)$$

cf. **Rokhlin's formula**, generalizing *Pesin's theorem* to intermittent dynamics (Korabel, Barkai, 2009; Howard, RK, tbp)

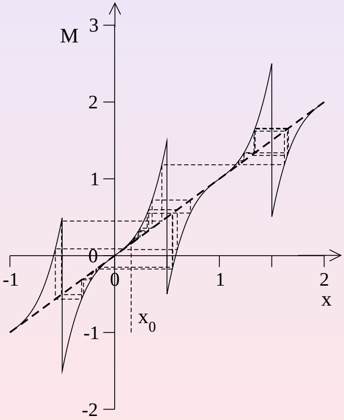
open question: Does there exist an anomalous escape rate formula for the *open* system?

note: conference on Weak Chaos, Infinite Ergodic Theory, and Anomalous Dynamics (MPIPKS Dresden, 2011)

An intermittent map with anomalous diffusion

continue map by $M(-x) = -M(x)$ and $M(x+1) = M(x) + 1$:

(Geisel, Thomae, 1984; Zumofen, Klafter, 1993)



deterministic random walk on the line; classify diffusion in terms of the mean square displacement

$$\left\langle x^2 \right\rangle = K\, n^\alpha \; (n \to \infty)$$

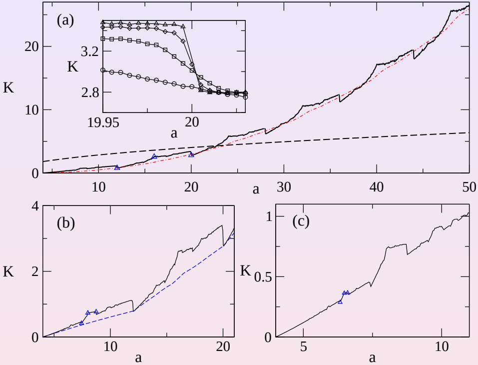
if $\alpha \neq 1$ one speaks of **anomalous diffusion**; here one finds

$$\alpha = \begin{cases} 1, & 1 \leq z \leq 2 \\ \frac{1}{z-1} < 1, & 2 < z \end{cases}$$

focus on generalized diffusion coefficient $K = K(z, a)$

Parameter dependent anomalous diffusion

$K(z=3,a)$ for $M(x) = x + ax^3$ from computer simulations:



Korabel, R.K. et al., 2005

- $\exists$ fractal structure
- $K(a)$ conjectured to be discontinuous (inset) on dense set
- comparison with stochastic theory, see dashed lines

CTRW theory I: Montroll-Weiss equation

Montroll, Weiss, Scher, 1973:

master equation for a stochastic process defined by *waiting time distribution* $w(t)$ and *distribution of jumps* $\lambda(x)$:

$$\varrho(x,t) = \int_{-\infty}^{\infty} dx' \lambda(x-x') \int_0^t dt' \, w(t-t') \, \varrho(x',t') + \\ +(1-\int_0^t dt' w(t'))\delta(x)$$

structure: jump + no jump for particle starting at $(x,t)=(0,0)$

$\hat{\text{F}}$ourier-$\tilde{\text{L}}$aplace transform yields **Montroll-Weiss eqn (1965)**

$$\hat{\tilde{\varrho}}(k,s) = \frac{1-\tilde{w}(s)}{s} \frac{1}{1-\hat{\lambda}(k)\tilde{w}(s)}$$

with mean square displacement $\langle \tilde{x^2}(s) \rangle = -\left.\frac{\partial^2 \hat{\tilde{\varrho}}(k,s)}{\partial k^2}\right|_{k=0}$

CTRW theory II: application to maps

apply CTRW to maps (Klafter, Geisel, 1984ff): need $w(t), \lambda(x)$

- continuous-time approximation for the PM-map

$$x_{n+1} - x_n \simeq \frac{dx}{dt} = ax^z \, , \quad x \ll 1$$

solve for $x(t)$ with initial condition $x(0) = x_0$, define jump as $x(t) = 1$, solve for $t(x_0)$ and compute $w(t) \simeq \varrho_{in}(x_0) \left| \frac{dx_0}{dt} \right|$ by assuming uniform density of injection points, $\varrho_{in}(x_0) \simeq 1$

- (revised) ansatz for jumps:

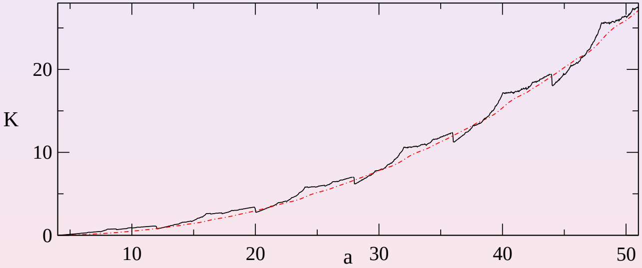
$$\lambda(x) = \frac{p}{2}\delta(|x| - \ell) + (1-p)\delta(x)$$

with jump length ℓ, escape probability
$p := 2(\frac{1}{2} - x_c)$, $M(x_c) := 1$
CTRW machinery . . . yields exactly

$$K = p\ell^2 \begin{cases} \frac{a^\gamma \sin(\pi\gamma)}{\pi\gamma^{1+\gamma}}, & 0 < \gamma < 1 \\ a\frac{\gamma-1}{\gamma}, & \gamma \geq 1 \end{cases} \quad , \quad \gamma := 1/(z-1) \, , \; z > 1$$

Anomalous random walk solution

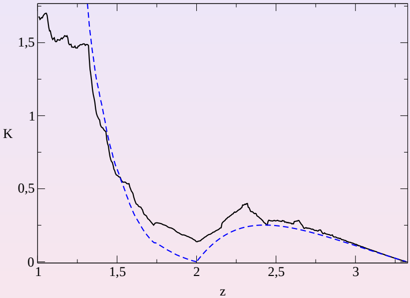
define average jump length $\ell := < |M(x) - x| >_{\varrho_0=1}$:
for $z = 3$ we get $K(a) \sim a^{5/2}$



CTRW yields **anomalous drunken sailor solution**, which correctly describes the coarse scale behaviour of $K(3, a)$

Dynamical phase transition to anomalous diffusion

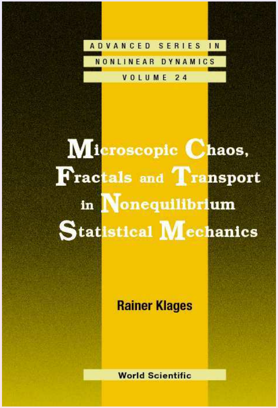
compare CTRW approximation (blue line) with simulation results for $K(z,5)$:



$\exists$ **full suppression of diffusion** due to logarithmic corrections

$$< x^2 > \sim \begin{cases} n/\ln n, n < n_{cr} \text{ and } \sim n, n > n_{cr}, & z < 2 \\ n/\ln n, & z = 2 \\ n^{\alpha}/\ln n, n < \tilde{n}_{cr} \text{ and } \sim n^{\alpha}, n > \tilde{n}_{cr}, & z > 2 \end{cases}$$

Reference



see Part 1 of this book