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

Rainer Klages

Queen Mary University of London, School of Mathematical Sciences

Wchaos11, MPIPKS Dresden, 11 August 2011

Setting the scene

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

⇨ theory of nonequilibrium statistical physics starting from microscopic chaos?

approach should be particularly useful for

'small' nonlinear systems

Outline

focus on **deterministic random walks on the line**

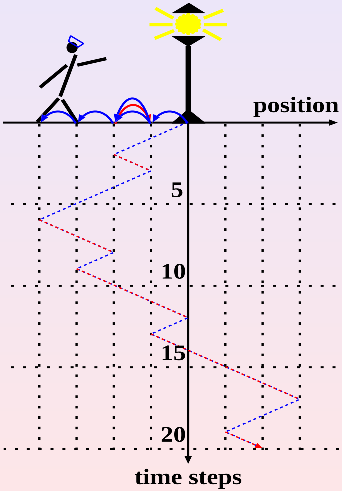
two lectures:

1. **Normal deterministic diffusion**
   two methods for two maps: Taylor-Green-Kubo and escape rate approach

2. **Anomalous (deterministic) diffusion**
   subdiffusion in a weakly chaotic map: CTRW theory and a fractional diffusion equation; fluctuation relations for anomalous stochastic processes

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 (coin tossing)
- 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 $< \dots > := \int dx \ \varrho(x) \dots$ of positions $x = x_0 \ , \ x \in \mathbb{R}$

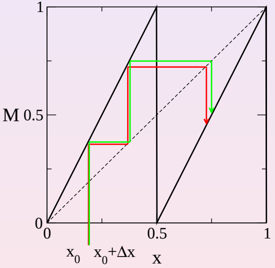
- for *sailor:* $D = s^2/2$

A simple chaotic map

problem: diffusion in chaotic dynamical systems?

brief reminder:

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



is **chaotic** with Ljapunov exponent $\lambda = \ln 2 > 0$: deterministic map that exhibits a lot of 'nice' dynamical systems properties

A deterministic random walk

study **diffusion** in the piecewise linear deterministic map

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

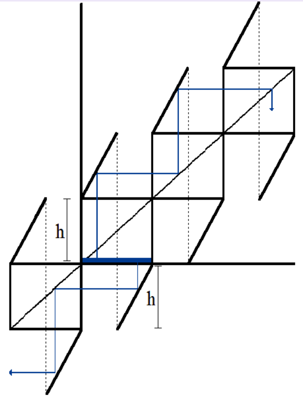
lifted onto the real line by

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

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

deterministic random walk generated by

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



Geisel/Grossmann/Kapral (1982)

Deterministic diffusion

two basic questions:

- Does this map exhibit diffusion?

  yes: Keller (1980), Hofbauer, Keller (1982)

- Can one calculate the diffusion coefficient $D(h)$?

  $\exists$ many different methods (analytically exact results in Groeneveld, RK (2002); Cristadoro (2006))

here two methods for two different maps:

1. Taylor-Green-Kubo approach (Knight, RK, 2011)
2. escape rate theory for diffusion (Gaspard, Nicolis, 1990)

Taylor-Green-Kubo approach

start from 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 of $m_h(x) := M_h(x) \bmod 1$; 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: (coding!)

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 $dt(x)/dx := j_0(x)$; **(picture!)** can be solved to

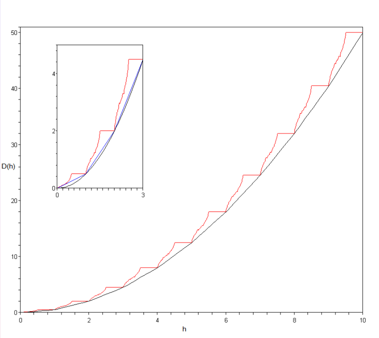
$$T_h^n(x) = \sum_{k=0}^{n} \frac{1}{2^k} t(m_h(x))$$

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

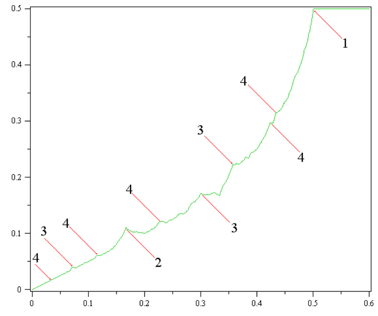
$$\boxed{D(h) = \frac{\lceil h \rceil^2}{2} + \left(\frac{1-\hat{h}}{2}\right)(1 - 2\lceil h \rceil) + T_h\left(\hat{h}\right)}$$

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



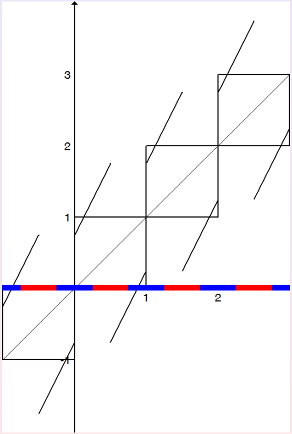
on large scales we recover the drunken sailor's result, $D(h) \sim h^2/2 \; (h \gg 1)$



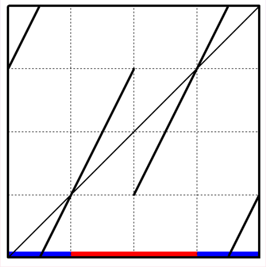
on small scales, $D(h)$ is *partially* a fractal function (due to topological instability under parameter variation)

Why the plateau regions?

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

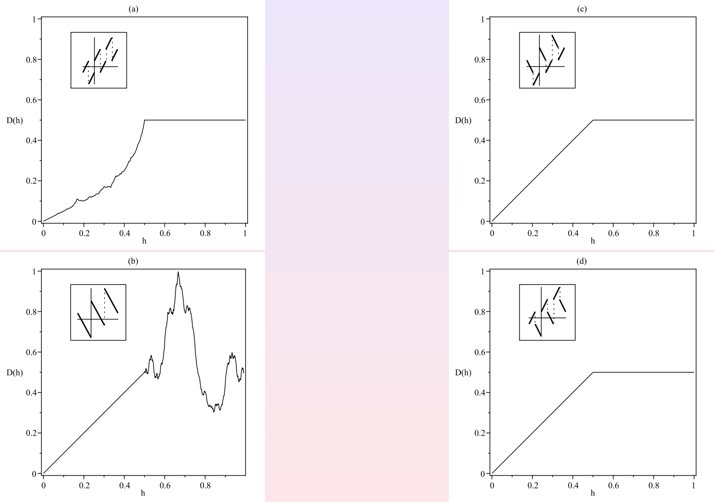


The phase space is split up into two invariant sets, see the mod 1 map:



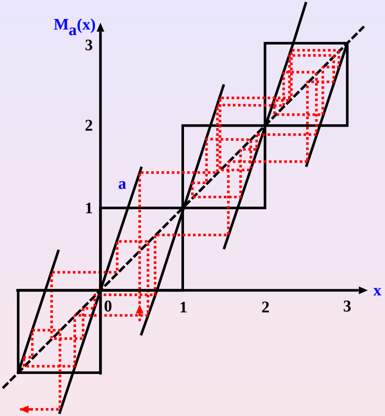
For a *uniform initial density*, the diffusion coefficient is calculated to $D(h) = D(h) + D(h) = (1 - h) + (h - \frac{1}{2}) = \frac{1}{2}$.

Outlook



see poster by Georgie or Knight, RK (2011)

A slightly more complicated diffusive map



(for slope $a \notin \mathbb{N}$, the invariant density for $M_a(x) \mod 1$ is *not uniform*)

goal: derive an exact relation between the diffusion coefficient $D(a)$ and dynamical systems quantities

Escape rate formalism, Step 1: diffusion equation

solve the ordinary one-dimensional **diffusion equation**

$$\frac{\partial n}{\partial t} = D\,\frac{\partial^2 n}{\partial x^2}$$

with $n = n(x,t)$ distribution function at point x and time t; D defines the diffusion coefficient

solution for absorbing boundaries, $n(0,t) = n(L,t) = 0$:

$$n(x,t) = \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\pi m}{L}\right)^2 Dt\right) a_m \sin\left(\frac{\pi m}{L} x\right)$$

with a_m determined by the initial density $n(x,0)$

Q: do we get the same for our deterministic chaotic model?

Escape rate formalism, Step 2: FP equation

solve the **Frobenius-Perron** (Liouville) **equation**

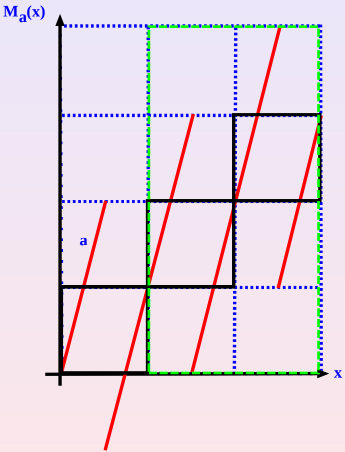
$$\varrho_{n+1}(x) = \sum_{x=M_a(x^i)} \varrho_n(x^i)|M_a'(x^i)|^{-1}$$

for the probability density $\varrho_n(x)$ of $M_a(x)$

• **basic idea:** construct FP-operator as transition matrix $T(a)$ applied to column vector $\underline{\varrho}_n$ of the probability density $\varrho_n(x)$:

$$\underline{\varrho}_{n+1} = \frac{1}{a} T(a) \, \underline{\varrho}_n$$

example: construction of T for $a = 4$



Markov partition

$$T(4) = \begin{pmatrix} & \vdots & \vdots & \\ \cdots & 1 & 0 & \cdots \\ & 2 & 1 & \\ & 1 & 2 & \\ \cdots & 0 & 1 & \cdots \\ & \vdots & \vdots & \end{pmatrix}$$

topological transition matrix

• solve the FP-equation: let $T(4)\,|\phi_m(x)>=\chi_m(4)\,|\phi_m(x)>$ be the eigenvalue problem of $T(4)$ with eigenvalues $\chi_m(4)$ and eigenvectors $|\phi_m(x)>$

$|\rho_{n+1}(x)>=\underline{\varrho}_{n+1}$ by spectral decomposition:

$$
\begin{aligned}
|\rho_{n+1}(x)> &= \frac{1}{4}\sum_{m=1}^{L}\chi_m(4)\,|\phi_m(x)><\phi_m(x)|\rho_n(x)> \\
&= \sum_{m=1}^{L}\exp\left(-n\ln\frac{4}{\chi_m(4)}\right)|\phi_m(x)><\phi_m(x)|\rho_0(x)>
\end{aligned}
$$

for initial probability density vector $|\rho_0(x)>$

• solve the eigenvalue problem for absorbing boundaries, $\varrho_n(0)=\varrho_n(L)$: analytical solution only available in special cases, as for $a=4$

Escape rate formalism, Step 3: match the solutions

match the largest eigenmodes in the limit of chain length $L \to \infty$ and time $n \to \infty$

- **diffusion equation:** $n(x,t) \simeq \exp\left(-\left(\frac{\pi}{L}\right)^2 Dt\right) A \sin\left(\frac{\pi}{L}x\right)$
- **FP-equation:** $\rho_{n+1}(x) \simeq \exp\left(-\gamma(4)n\right)\tilde{A} \sin\left(\frac{\pi}{L+1}k\right)$

$$k = 1, \ldots, L \quad , \quad k - 1 < x \leq k \ ,$$

where $\gamma(4) = \ln \frac{4}{\chi_{max}(4)}$ is the escape rate with $\chi_{max}(4) = 2 + 2\cos\frac{\pi}{L+1}$ as the largest eigenvalue of $T(4)$

- **match:** $$D(4) = \left(\frac{L}{\pi}\right)^2 \gamma(4) \to \frac{1}{4} \quad (L \to \infty)$$

exact method to calculate $D(4)$; result is identical to random walk solution :-|

Escape rate formula for diffusion

establish relation between diffusion coefficient and dynamical systems quantities: it was

$$D = \lim_{L\to\infty} \left(\frac{L}{\pi}\right)^2 \gamma$$

with

$$\gamma = \ln |M'(x)| - \ln \chi_{max}$$

cp. with escape rate formula from Phil's talk:

$$\gamma = \lambda(\mathcal{R}_L) - h_{KS}(\mathcal{R}_L)$$

general result:

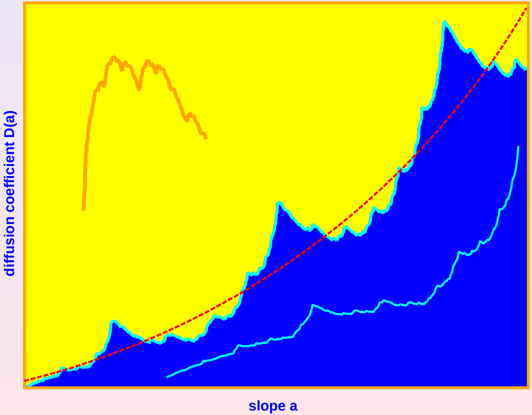
$$\boxed{D = \lim_{L\to\infty} \left(\frac{L}{\pi}\right)^2 [\lambda(\mathcal{R}_L) - h_{KS}(\mathcal{R}_L)]}$$

escape rate formula for diffusion

Gaspard, Nicolis, Dorfman (1990ff)

Parameter-dependent deterministic diffusion

result for the parameter dependent diffusion coefficient $D(a)$:

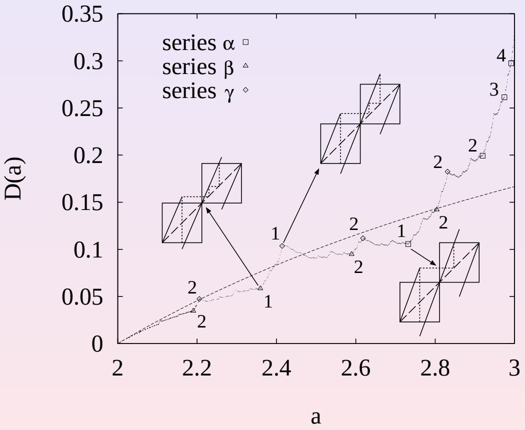


RK, Dorfman (1995)

compare again diffusion of drunken sailor with chaotic model

Physical explanation of the fractal structure

blowup of the initial region of $D(a)$:



local extrema are generated by specific sequences of **correlated microscopic scattering processes**

$D(a)$ is actually a very strange fractal:

Proposition

For the family of maps M_a there is a constant $C > 0$ such that the diffusion coefficient $D(a)$ satisfies

$$|D(a) - D(a')| \leq C|a - a'|(1 + |\log|a - a'||)^2$$

i.e., $D(a)$ is *log-Lipschitz continuous*. This implies for box counting

$$N(\epsilon) \leq C\epsilon^{-1}(1 - \ln\epsilon)^2 \ , \ \epsilon \ll 1$$

and

Corollary

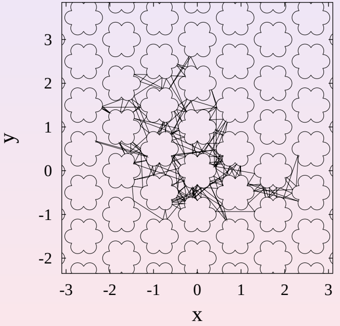
The graph of D has box- and Hausdorff-dimension 1.

note: numerics suggests $N(\epsilon) = C_1\epsilon^{-1}(1 + C_2 \ln\epsilon)^{\alpha}$ with a *locally varying* exponent $0 \leq \alpha \leq 1.2$

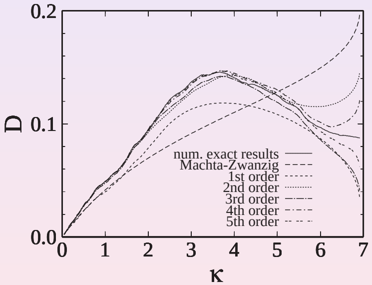
Keller, Howard, RK (2008)

Outlook: diffusion in billiards

flower-shaped scatterers with petals of curvature κ:



simulation results for the diffusion coefficient (with truncated TGK analysis):



Harayama, R.K., Gaspard (2002)

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

References

- **TGK approach:**

G.Knight, RK, Nonlinearity **24**, 227 (2011)

- **ecape rate approach:**

RK, *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