Stochastic modeling of diffusion in dynamical systems: three examples

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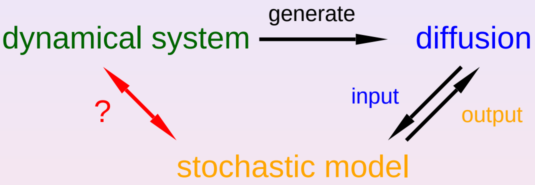
Outline

1. **Motivation:**
   dynamical systems, diffusion and stochastic modeling
2. **Diffusion in three different dynamical systems:**
   1. non-chaotic ‘slicer’ map
   2. soft periodic Lorentz gas
   3. a simple random dynamical system
3. **Conclusion:**
   successes, failures and pitfalls for these three examples when relating the above three layers to each other

Dynamical systems, diffusion and stochastic modeling

theme of this talk:

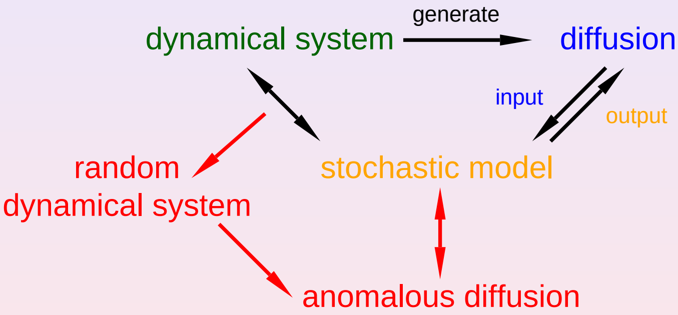


two questions:

1. what type of diffusion is generated by a dynamical system?
2. can it be reproduced by some stochastic model?

Random Dyn. Systems and Anomalous Dynamics

relation to workshop theme:



will be illustrated by three examples

Basic diffusive setup

- in the following only diffusion in one dimension
- key quantity: **mean square displacement**

$$< x^2 >:= \int dx\ x^2 \rho(x,t) \sim t^\gamma$$

- **note:** three basic types of diffusion
  1. there is not only 'Brownian' (normal) diffusion with $\gamma = 1$ but also **anomalous diffusion**:
  2. subdiffusion with $\gamma < 1$ and
  3. superdiffusion with $\gamma > 1$

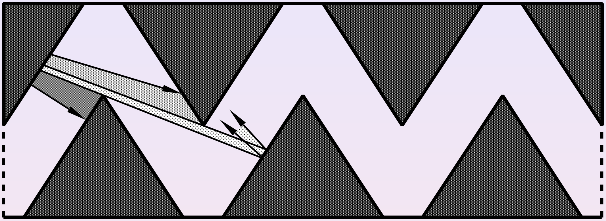
(plus more exotic types)

I. The slicer map

together with:

L.Salari and L.Rondoni (Torino)
C.Giberti (Reggio E.)

Motivation: diffusion in polygonal billiards

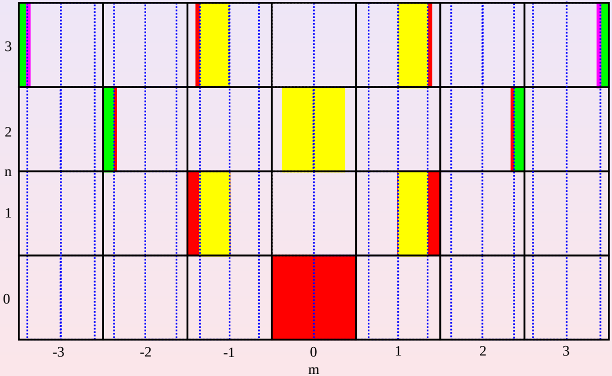


Zaslavsky et al. (2001), Jepps et al. (2006)

- zero Lyapunov exponent: different points separate *linearly* but not *exponentially* in time, hence non-chaotic dynamics
- mean square displacement from simulations: sub-, super- or normal diffusion depending on parameters, with partially conflicting results (Alonso / Jepps / Sanders et al., 2002ff)

Pictorial construction

a one-dimensional ‘random walk-like’ but fully deterministic system; diffusion of a density of points from uniform initial density in **space (m) - discrete time (n) diagram**:



slicers (blue lines) split the density and move parts around; no stretching, hence zero Lyapunov exponent: **no chaos!**

Formal definition

• consider a chain of intervals $\widehat{M} := M \times \mathbb{Z}$, $M := [0,1]$ with point $\widehat{X} = (x,m)$ in $\widehat{M}$, where $\widehat{M}_m := M \times \{m\}$ is the m-th cell of $\widehat{M}$

• subdivide each $\widehat{M}_m$ in subintervals, separated by points called slicers: $\{1/2\} \times \{m\}$, $\{\ell_m\} \times \{m\}$, $\{1-\ell_m\} \times \{m\}$, where $0 < \ell_m < 1/2$ for every $m \in \mathbb{Z}$ with

power law $\ell_m(\alpha) = \frac{1}{\left(|m|+2^{1/\alpha}\right)^{\alpha}}$, $\alpha > 0$

• slicer map: $S : \widehat{M} \to \widehat{M}$, $\widehat{X}_{n+1} = S(\widehat{X}_n)$, $n \in \mathbb{N}$ with

$$S(x,m) = \begin{cases} (x, m-1) & \text{if } 0 \le x < \ell_m \text{ or } \frac{1}{2} < x \le 1 - \ell_m, \\ (x, m+1) & \text{if } \ell_m \le x \le \frac{1}{2} \text{ or } 1 - \ell_m < x \le 1. \end{cases}$$

$\Rightarrow$ interval exchange transformation lifted onto the real line

Main result: diffusive properties

Proposition: Salari et al., 2015

Given $\alpha \geq 0$ and a uniform initial distribution in $\widehat{M}_0$, we have

1. $\alpha = 0$: ballistic motion with MSD $\langle \widehat{X}_n^2 \rangle \sim n^2$
2. $0 < \alpha < 1$: superdiffusion with MSD $\langle \widehat{X}_n^2 \rangle \sim n^{2-\alpha}$
3. $\alpha = 1$: normal diffusion with linear MSD $\langle \widehat{X}_n^2 \rangle \sim n$
   non-chaotic normal diffusion with non-Gaussian density
4. $1 < \alpha < 2$: subdiffusion with MSD $\langle \widehat{X}_n^2 \rangle \sim n^{2-\alpha}$
   subdiffusion with ballistic peaks
5. $\alpha = 2$: logarithmic subdiffusion with MSD $\langle \widehat{X}_n^2 \rangle \sim \log n$
   a bit exotic
6. $\alpha > 2$: localisation in the MSD with $\langle \widehat{X}_n^2 \rangle \sim const.$
   non-trivial phenomenon

nb: higher order moments $\langle \widehat{X}_n^p \rangle$ can also be calculated

Matching to stochastic dynamics?

curiously, the slicer moments bear formal similarity with **different stochastic models**:

- one-dimensional stochastic Lévy Lorentz gas:
  matching of all moments in the superdiffusive regime by a non-trivial scaling
- Lévy walk modeled by CTRW theory:
  matching of all moments in the superdiffusive regime by a *different* simple scaling
- correlated Gaussian stochastic process:
  same MSD in the subdiffusive regime

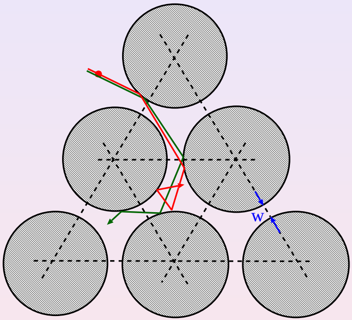
$\Rightarrow$ slicer might help to explain a **controversy about different stochastic models for diffusion in polygonal billiards**

II. The soft Lorentz gas

together with:

S.S.G.Gallegos (London)
J.Solanpäa, M.Sarvilahti and E.Räsänen (Tampere)

Review: The periodic Lorentz gas



Lorentz (1905)

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, cf. density of scatterers

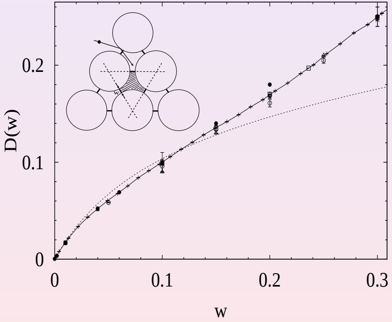
paradigmatic example of a **chaotic** Hamiltonian particle billiard:
$\exists$ positive Ljapunov exponent;
$\exists$ diffusion in certain range of w
Bunimovich, Sinai (1980)

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

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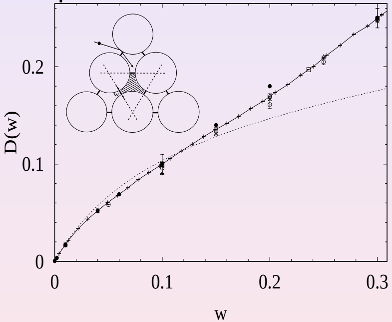
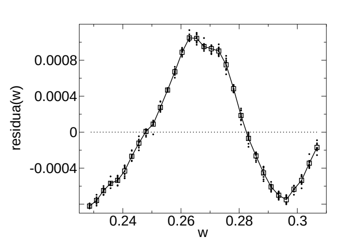


residua for large w:



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

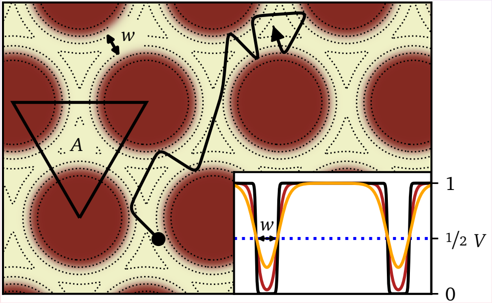
Question: What happens to $D(w)$ if one softens the scatterers?

Our model

We choose overlapping Fermi potentials

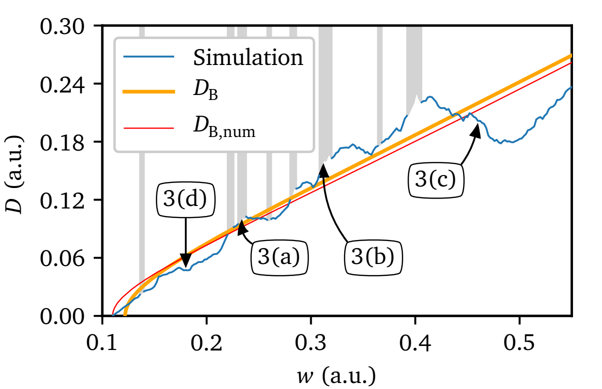
$$V(\mathbf{r}) = \frac{1}{1 + \exp\left(\frac{|\mathbf{r}| - r_o}{\sigma}\right)}$$

with softness parameter σ and total energy $E = 1/2$



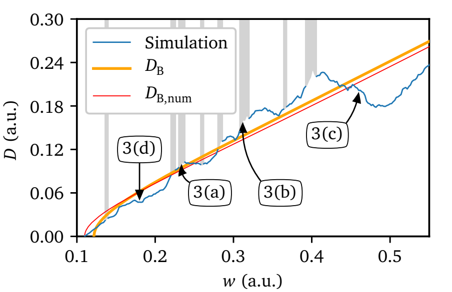
diffusion coefficient $D(w)$ computed with software package *bill2d* by Solanpää et al. (2016)

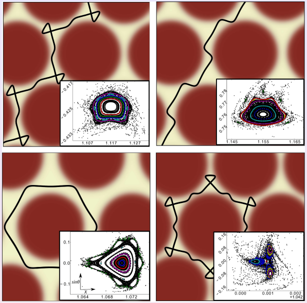
Results: Diffusion coefficient D(w)



- $D(w)$ is a highly irregular function of the control parameter
- the coarse form matches to a Boltzmann approximation $D_B(w) = \ell_c^2/(4\tau_c)$ (orange analytical, red numerical)
- there are parameter regions exhibiting superdiffusion

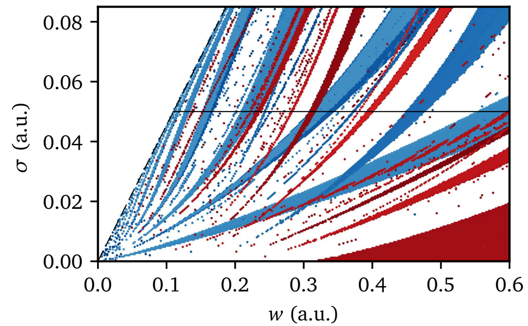
Explanations: diffusion and periodic orbits





- extrema in $D(w)$ related to islands of periodicity in mixed phase space (Geisel et al., 1987ff; Zaslavsky, 2002)
- two types: ballistic orbits lead to superdiffusion, localised orbits decrease normal diffusion
- mathematical conjecture that islands are dense in parameters under smoothening (Turaev, Rom-Kedar, 1998)

Periodic orbits in parameter space



blue: localised; red ballistic periodic orbits

- there is a very regular structure of periodic orbits underlying the highly irregular $D(W)$
- no fit with simple functional forms
- open question to build a theory for these tongues

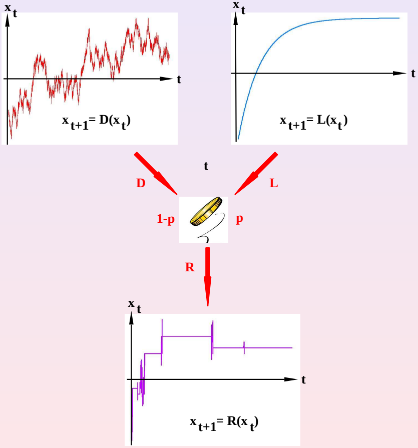
III. A random dynamical system

together with:

Y.Sato (Hokkaido)

Constructing a random dynamical system

three time series for position x_t of a particle at discrete time t:



- *upper left:* deterministic dynamical system D yielding normal diffusion
- *upper right:* deterministic dynamical system L where all particles localize in space.
- *bottom:* **random dynamical system** R that mixes these two types of dynamics at time t with probability p; the result is intermittent motion

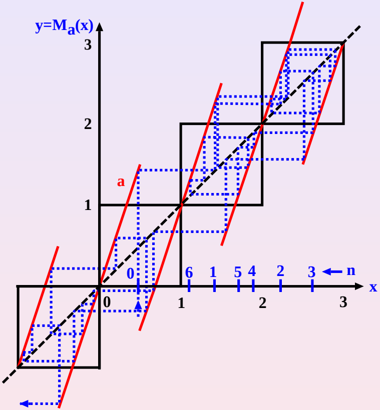
Our model

equation of motion
$x_{t+1} = M_a(x_t)$ with discrete time
$t \in \mathbb{N}_0$, $a > 0$ and
one-dimensional piecewise
linear map

$$M_a(x) = \begin{cases} ax \,, 0 \le x < \frac{1}{2} \\ ax + 1 - a \,, \frac{1}{2} \le x < 1 \end{cases}$$

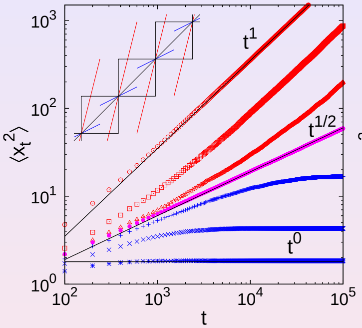
lift $M_a(x+1) = M_a(x) + 1$;
Lyapunov exponent $\lambda(a) = \ln a$

RK, J.R.Dorfman, 1995



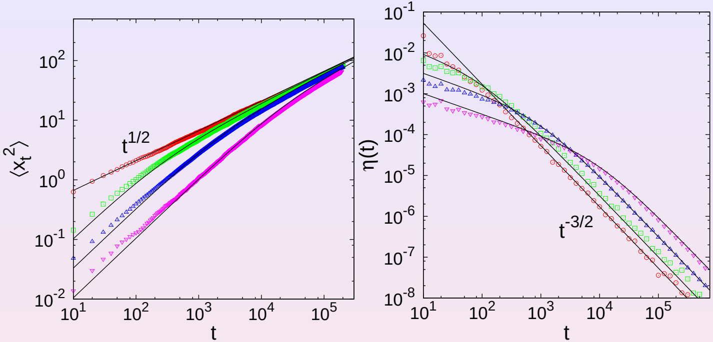
random map $R = M_a(x)$: at any t choose a iid with probability $p \in [0,1]$ from $a = 1/2$ and with $1 - p$ from $a = 4$

Diffusion in a simple random dynamical system



- *left:* $\langle x_t^2 \rangle$ for $p = 0.6, \ldots, 0.7$ (top to bottom); subdiffusion with zero Lyapunov exponent at $p_c = 2/3$
- *right:* $\langle x_t^2 \rangle$ at p_c with *same* random sequence for *each* particle (colors), cp. to *different* random sequence (**black**); MSD is a random variable breaking self-averaging and ergodicity

Ageing and weak ergodicity breaking



• *left:* $\langle x_t^2 \rangle$ at p_c by starting the computations after different ageing times $t_a = 0, 10^2, 10^3, 10^4$ (top to bottom) displays ageing, cp. to CTRW theory (Barkai, 2003; bold lines)

• *right:* corresponding waiting time distribution $\eta(t)$ (for particles leaving a unit cell at t_a), again matching to CTRW theory

• both results imply weak ergodicity breaking (Bouchaud, 1992)

Connection with dynamical systems theory

- mixing 'expanding'/chaotic with contracting/non-chaotic dynamics randomly in time generates intermittent motion
- the underlying microscopic mechanism is called on-off intermittency (Pikovsky (1984), Fujisaka et al. (1985)); transition called blowout bifurcation (Ott et al. (1994))

Summary

- **central theme:** interplay between *dynamical systems, diffusion and stochastic modeling*
- **main results:**
  1. (random) dynamical systems can feature *novel types of (anomalous) diffusion*
  2. naive matching to stochastic models can be misleading and difficult
- **outlook:** perhaps dynamical systems theory can inspire stochastic theory to invent new stochastic processes?

References

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