Stochastic modeling of diffusion in dynamical systems: two examples

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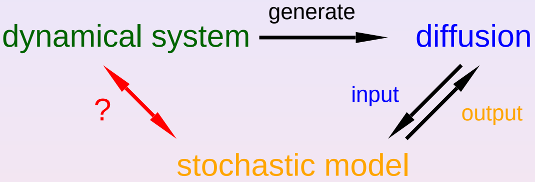
Outline

- **theme of this talk:**

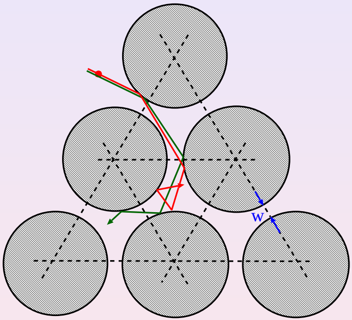


- **two questions:**
  1. what type of diffusion is generated by a dynamical system?
  2. can it be reproduced by some stochastic model?

- **two examples:** successes and limitations
  1. diffusion in a soft Lorentz gas (parts 1 - 3)
  2. a random dynamical system (part 4)

1. The soft Lorentz gas

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

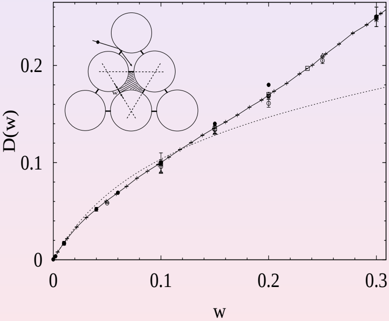
paradigmatic example of a **chaotic** Hamiltonian particle billiard:
$\exists$ positive Lyapunov exponent;
$\exists$ diffusion in certain range of w
Bunimovich, Sinai (1980)

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 (left): random walk approx. by Machta, Zwanzig (1983), $D_{\mathrm{MZ}}(w) = \ell^2/4\tau$ with ℓ distance between 'traps', τ escape time

Diffusion coefficient for the periodic Lorentz gas

diffusion coefficient $D(w) = \lim_{t\to\infty} < (\mathbf{x}(t) - \mathbf{x}(0))^2 > /(4t)$

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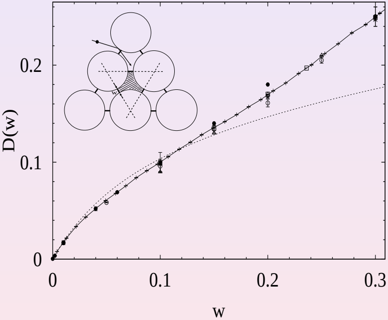
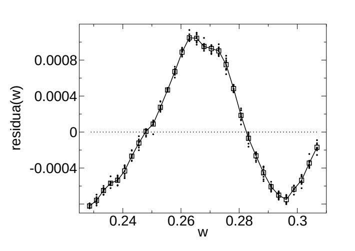


residua for large w:

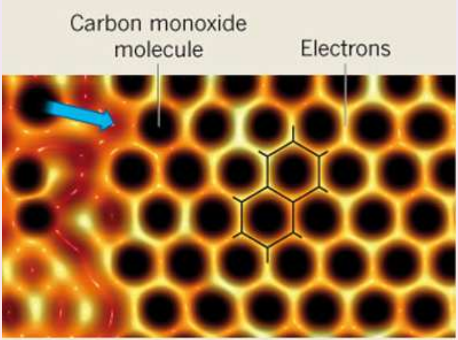


- dots (left): random walk approx. by Machta, Zwanzig (1983), $D_{\mathrm{MZ}}(w) = \ell^2/4\tau$ with ℓ distance between 'traps', τ escape time
- $\exists$ irregularities on fine scales; RK, Dellago (2000)

Diffusion in soft Lorentz gases

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

Motivation: model diffusion of electrons in artificial graphene, here between CO molecules on a copper surface:



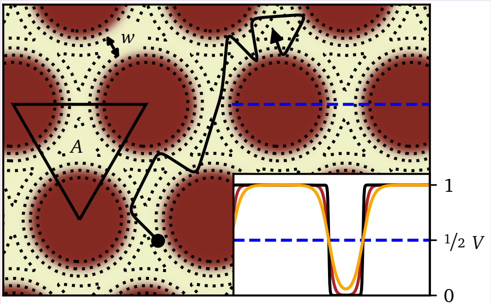
Gomes et al., Nature (2012)

Our model

We choose overlapping Fermi potentials

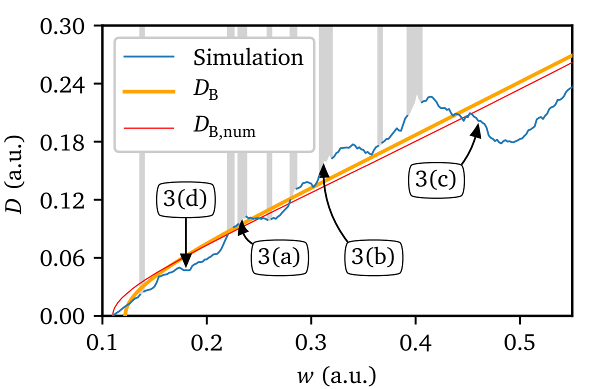
$$V(\mathbf{r}) = \frac{1}{1+\exp\left(\frac{|\mathbf{r}|-r_0}{\sigma}\right)}\ ,\ r_0 = 1$$

with softness parameter σ and total energy E



3 parameters: w, E, σ; diffusion coefficient $D(w,E)$ computed with software package *bill2d* by Solanpää et al. (2016)

Diffusion coefficient D(w) for $\sigma = 0.05$ and E=1/2



- $D(w)$ is a highly irregular function of w
- the coarse form matches to a *Boltzmann approximation* (orange analytical, red numerical)
- there are parameter regions exhibiting superdiffusion

Boltzmann approximation for diffusion

$$D_B(w) = \frac{\ell_c^2}{4\tau_c} \, ,$$

where ℓ_c is the collision length of a particle hitting the equipotential line and τ_c the collision time

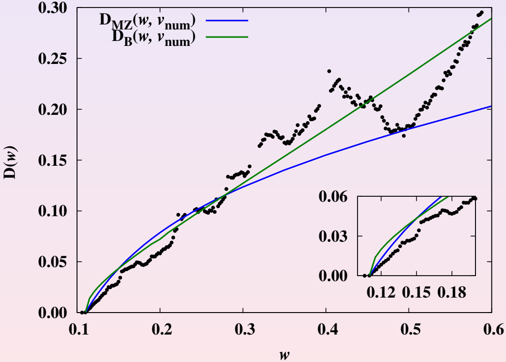
- τ_c calculated by a simple (MZ) phase space argument
- ℓ_c eliminated by defining an average speed $v = \ell_c/\tau_c$ yielding

$$D_B(w) = \frac{v^2\tau_c}{4}$$

- two approximations for v when leaving a trap:
  1. analytical by an average potential
  2. numerical by the correct average speed

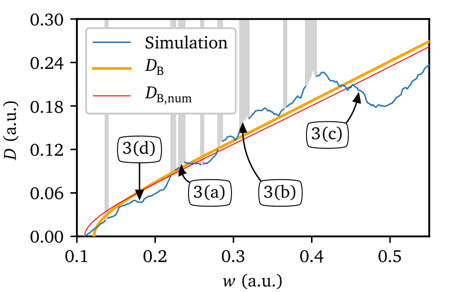
Crossover between different random walks

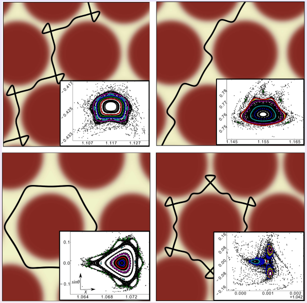
comparison between a MZ approximation D_{MZ} suitably adapted to the soft Lorentz gas and D_B:



D_{MZ} better at the onset of diffusion with crossover to D_B for larger w; general feature (RK, 1997; RK, Dellago, 2000)

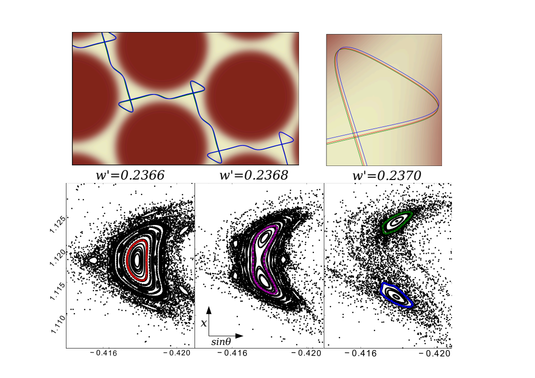
Anomalous diffusion and periodic orbits





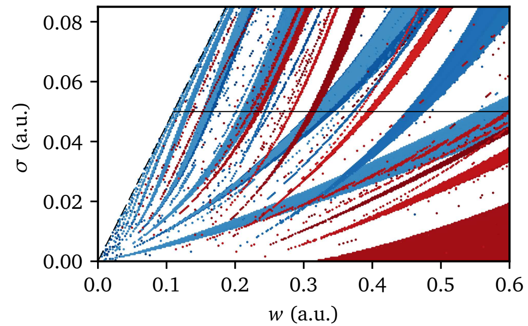
- extrema in $D(w)$ related to islands of periodicity in mixed phase space (Geisel et al., 1987ff; Zaslavsky, 2002)
- two types: ballistic orbits lead to superdiffusion, localised orbits decrease normal diffusion
- mathematical conjecture that islands are dense in parameters under smoothing (Turaev,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

Bifurcations



- complicated bifurcation scenarios determine the size of the anomalous parameter regions

Periodic orbits in parameter space

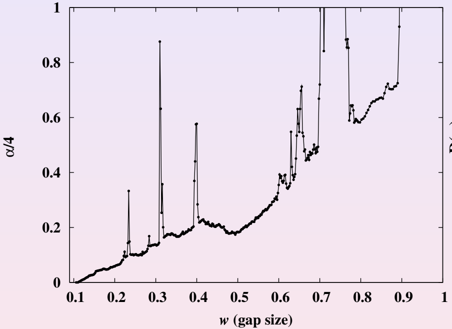


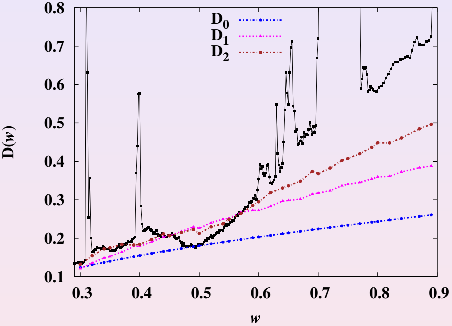
blue: localised; red ballistic periodic orbits

- 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

D(w) for larger w?

D(*w*) story not yet complete:

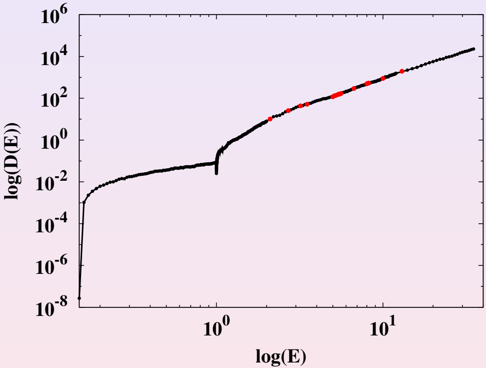




- after MZ and Boltzmann a third diffusive regime for larger *w*
- diffusion highly correlated therein: complicated scattering
- microscopic explanation by correlated random walk approximation (RK, Korabel, 2002)

Energy-dependent diffusion coefficient D(E)

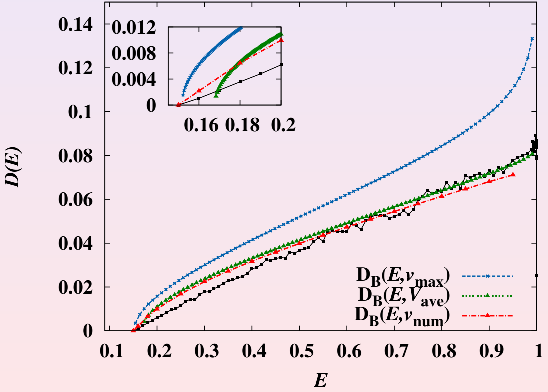
keep $w = 0.05$ constant at $\sigma = 0.01$ and vary the energy E:



There exist three different diffusive regimes for small, intermediate and large energies (plus superdiffusive regions, cf. red dots).

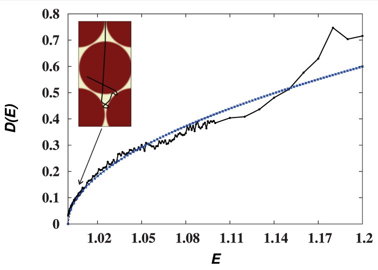
D(E) for small energies

A suitably worked out Boltzmann approximation $D_B(E)$ (here also for a maximum velocity) reproduces the low energy diffusion regime:



D(E) for intermediate energies

for energy $E = 1$ a particle can for the first time fly over the top of a potential:



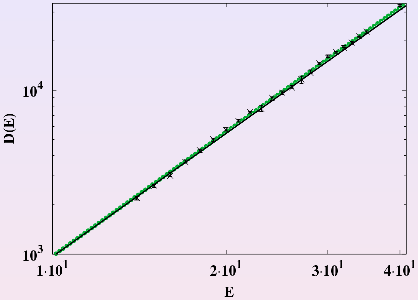
- full suppression of diffusion at $E = 1$
- each potential maximum becomes a trap, where the particle loses (all) kinetic energy

reproduced by a random walk approximation

$$D_s(E) = \ell^2/(4\tau(E))$$

with distance ℓ between potential maxima and escape time τ from a trap, calculated again by a phase space argument; yields $D_s =\sim \sqrt{E-1}$, cf. blue line above

D(E) for high energies

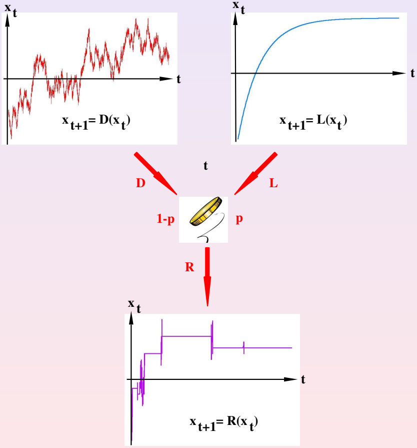


- *D*(*E*) increases as a power law with exponent 2.5
- predicted by high energy random walk approximation where particles travel over long distances before slightly changing direction (Aguer et al., 2010)
- for large energies superdiffusive parameter regions become ubiquitous

2. A random dynamical system

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

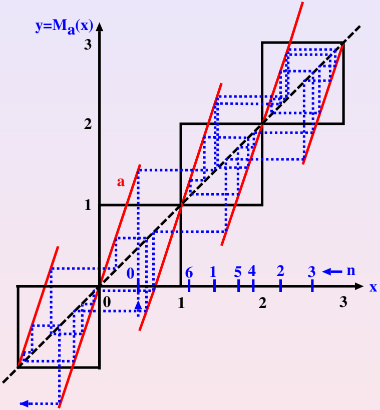
$x_{t+1} = M_a(x_t)$ with discrete time $t \in \mathbb{N}_0$, $a > 0$ and

one-dimensional piecewise linear map

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

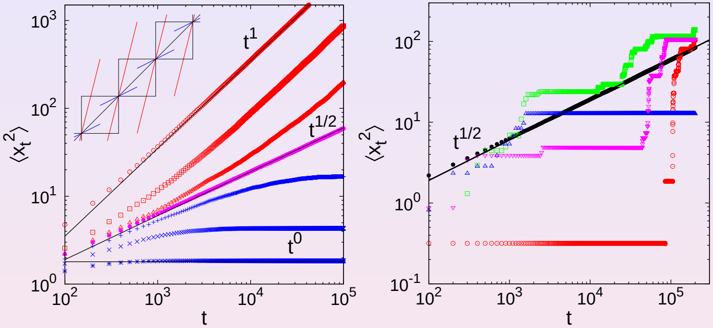
lift $M_a(x+1) = M_a(x) + 1$;

Lyapunov exponent $\lambda(a) = \ln a$



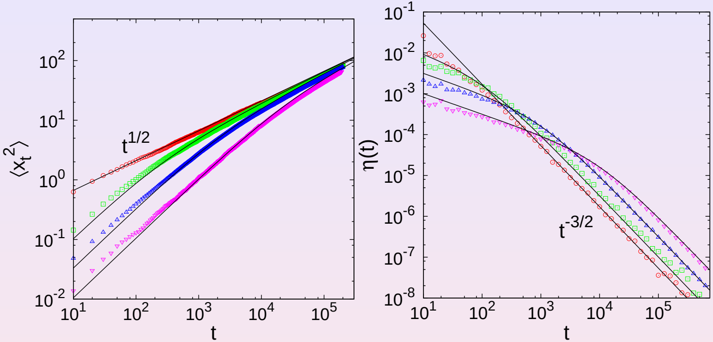
random map $R = M_a(x)$: at any t choose a iid with probability $p \in [0, 1]$ from $a = 1/2$ and with $1 - p$ from $a = 4$

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

1. **diffusion in a soft Lorentz gas:**
   - even at minimal softening the diffusion coefficient becomes a highly irregular curve under parameter variation with regions of superdiffusion
   - different diffusive regimes all reproduced by simple random walk approximations; fine structure related to periodic orbits
   - rigorous theory? measurements in experiments?
2. **random dynamical system:**
   - can generate subdiffusion at a zero Lyapunov exponent similar to CTRW theory
   - generality of this mechanism to generate anomalous diffusion?

Summary

- R.Klages et al., *Normal and anomalous diffusion in soft Lorentz gases*, in print for PRL

- S.S.Gil-Gallegos et al., *Energy-dependent diffusion in a soft periodic Lorentz gas*, to be published in EPJ-ST Special Issue (Feb. 2019)

- Y.Sato, R.Klages, *Anomalous diffusion in random dynamical systems*, to be resubmitted to PRL

all available on arXiv