How does a diffusion coefficient depend on size and position of a hole?

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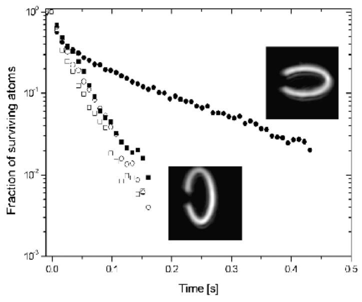
Outline

1. **escape of particles in billiards and maps**: from experiment to theory
2. **hole dependence of diffusion** in a simple chaotic map: from theory to experiment?

Motivation: Experiments on atom-optics billiards

ultracold atoms confined by a rapidly scanning *laser beam* generating *billiard-shaped potentials*

measure the decay of the number of atoms through a hole:

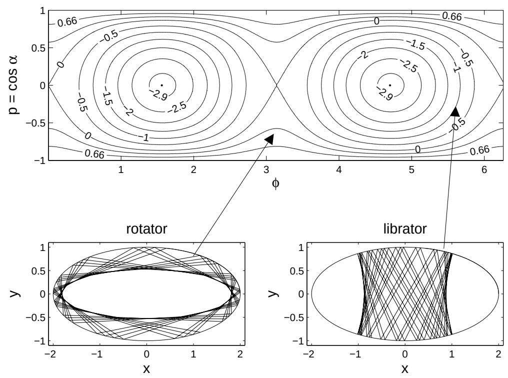


Friedmann et al., PRL (2001); see also Milner et al., PRL (2001)

⇒ **decay** depends on the **position of the hole**

Microscopic dynamics of particle billiards

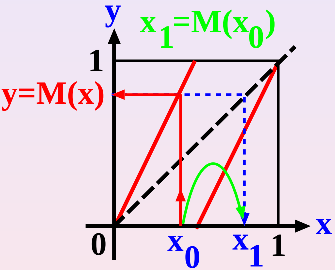
explanation: hole like a *scanning device* that samples different microscopic structures in different phase space regions



Lenz et al., PRE (2007)

Simplify the system

Instead of a particle billiard, consider a toy model: simple one-dimensional **deterministic map**



iterate steps on the unit interval in discrete time according to

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

as equation of motion with

$$\boxed{M(x) = 2x \bmod 1}$$

Bernoulli shift

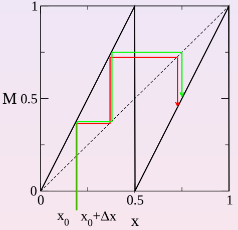
note: This dynamics can be mapped onto a stochastic *coin tossing sequence* (cf. random number generator)

Ljapunov exponents and periodic orbits

Bernoulli shift dynamics again: $x_n = 2x_{n-1} \bmod 1$

Iterate a small perturbation

$\Delta x_0 := \tilde{x}_0 - x_0 \ll 1$:

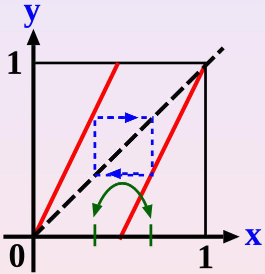


$$\Delta x_n = 2\Delta x_{n-1} = 2^n \Delta x_0$$
$$= e^{n \ln 2} \Delta x_0$$

Ljapunov exponent

$\lambda := \ln 2 > 0$

But there are also ...



... infinitely many **periodic orbits**, and they are dense on the unit interval.

Deterministic chaos

Definition of deterministic chaos according to Devaney (1989):

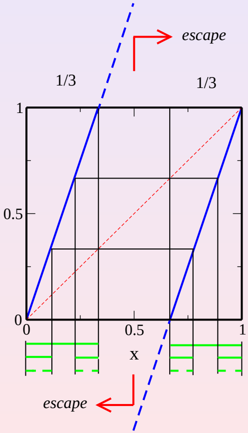
1. **irregularity:** There is sensitive dependence on initial conditions.
2. **regularity:** The periodic points are dense.
3. **indecomposability:** The system is topologically transitive.

The Bernoulli shift is **chaotic** in that sense.

(**nb:** 2 and 3 imply 1)

Hole and escape: a textbook problem

choose $M(x) = 3x \bmod 1$ and ‘dig a hole in the middle’:



- There is escape from a fractal Cantor set.
- The number of particles decays as $N_n = N_0 \exp(-\gamma n)$ with escape rate $\gamma = \ln(3/2)$.

see e.g. Ott, Chaos in dynamical systems (Cambridge, 2002)

Hole and escape revisited

Bunimovich, Yurchenko:

Where to place a hole to achieve a maximal escape rate?

(Isr.J.Math., submitted 2008, published 2011!)

Theorem for Bernoulli shift:

Consider holes at *different positions* but with *equal size*.
Find in each hole the *periodic point with minimal period*.
Then the escape will be **faster** through the hole where the minimal period is **bigger**.

Corollary:

The escape rate may be larger through smaller holes!

more general theorem (later on) by Keller, Liverani, JSP (2009)

Escape rate and diffusion coefficient

Solve the **one-dimensional diffusion equation**

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

for particle density $\varrho = \varrho(x,t)$ and diffusion coefficient D with absorbing boundary conditions $\varrho(0,t) = \varrho(L,t) = 0$:

$$\varrho(x,t) \simeq A \exp(-\gamma t) \sin\left(\frac{\pi}{L}x\right) \quad (t, L \to \infty)$$

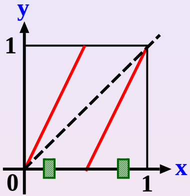
exponential decay with

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

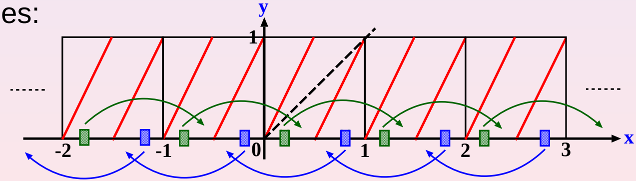
escape rate γ yields **diffusion coefficient** D

A deterministically diffusive map

- 'dig' symmetric holes into the Bernoulli shift:



- copy the unit cell spatially periodically, and couple the cells by the holes:



question: How does the diffusion coefficient of this model depend on size and position of a hole?

Computing hole-dependent diffusion coefficients

rewrite Einstein's formula for the diffusion coefficient

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

with equilibrium average $<\ldots>:=\int_0^1 dx\ \rho(x)\ldots\ ,\ x = x_0$ as

$$D_n = \frac{1}{2}\left\langle v_0^2 \right\rangle + \sum_{k=1}^{n} \left\langle v_0 v_k \right\rangle \to D \quad (n \to \infty)$$

Taylor-Green-Kubo formula

with integer velocities $v_k(x) = \lfloor x_{k+1} \rfloor - \lfloor x_k \rfloor$ at discrete time k

jumps between cells are captured by *fractal functions*

$$T(x) := \int_0^x d\tilde{x} \sum_{k=0}^{\infty} v_k(\tilde{x}) \ ,$$

as solutions of (*de Rham-type*) functional recursion relations

Computing hole-dependent diffusion coefficients

For the Bernoulli shift $M(x)$ the equilibrium density is $\rho(x) = 1$.

Define the coupling by creating a map $\tilde{M}(x) : [0,1] \to [-1,2]$:

- jump through *left* hole to the *right*: if $x \in [a_1, a_2]$, $0 < a_1 < a_2 \leq 0.5$ then $\tilde{M}(x) = M(x) + 1$ yielding $v_k(x) = 1$
- jump through *right* hole to the *left*: if $x \in [1 - a_1, 1 - a_2]$ then $\tilde{M}(x) = M(x) - 1$ yielding $v_k(x) = -1$
- otherwise no jump, $\tilde{M}(x) = M(x)$ yielding $v_k(x) = 0$

This map is copied periodically by $\tilde{M}(x+1) = \tilde{M}(x) + 1 \, , \; x \in \mathbb{R}$.

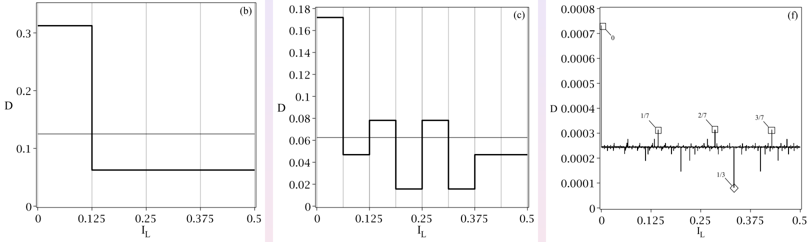
For this spatially extended model we obtain the exact result

$$\boxed{D = 2T(a_2) - 2T(a_1) - h \; ; \; h = a_2 - a_1}$$

Knight et al., preprint (2011)

Diffusion coefficient vs. hole position

Diffusion coefficient D as a function of the position of the left hole I_L of size $h = a_2 - a_1 = 1/2^s$, $s = 3, 4, 12$:



• (b), (c): for $I_L = [0.125, 0.25]$ it is $D = 1/16$, but for smaller hole $I_L = [0.125, 0.1875]$ we get larger $D = 5/64$

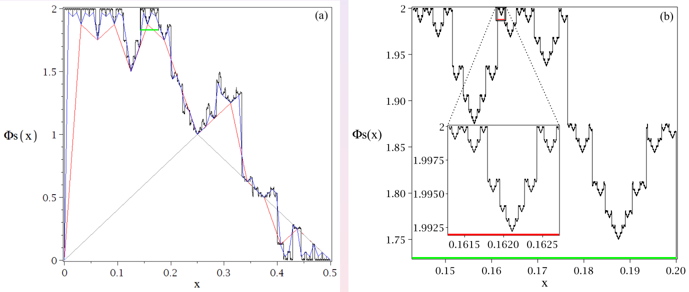
• (f): at $x = 0, 1/7, 2/7, 3/7$ particle keeps running through holes in one direction; at $x = 1/3$ particle jumps back and forth; these orbits dominate diffusion in the small hole limit

A fractal structure in the diffusion coefficient

resolve the irregular structure of the hole-dependent diffusion coefficient D by defining the cumulative function

$$\Phi_s(x) = 2^{s+1} \int_0^x \left(D(y) - 2^{-s}\right) dy$$

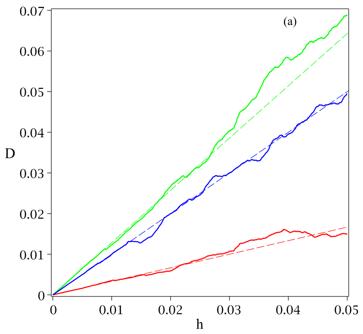
(subtract $< D_s >= 2^{-s}$ from $D(x)$ and scale with 2^{s+1})



- $\Phi_s(x)$ converges towards a fractal structure for large s
- this structure originates from the dense set of periodic orbits in $M(x)$ dominating diffusion

Diffusion for asymptotically small holes

center the hole on a standing, a non-periodic and a running orbit and let the hole size $h \to 0$:



dashed lines from analytical approximation for small h

$$D(h) \simeq \begin{cases} h\frac{1+2^{-p}}{1-2^{-p}} \,, & \text{running} \\ h\frac{1-2^{-p/2}}{1+2^{-p/2}} \,, & \text{standing} \\ h \,, & \text{non-periodic} \end{cases}$$

p : period of the orbit

- fractal parameter dependencies for $D(h)$ (RK, Dorfman, 1995)
- violation of the random walk approximation for small holes converging to periodic orbits!

Summary

How does a diffusion coefficient depend on **size** and **position** of a hole?

question answered for **deterministic dynamics** modeled by a simple **chaotic map**; two surprising results:

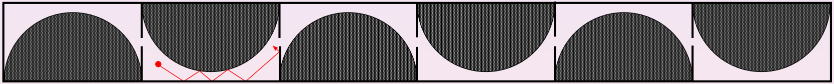
1. **size:** contrary to intuition, a smaller hole may yield a larger diffusion coefficient
2. **position:** violation of simple random walk approximation for the diffusion coefficient if the hole converges to a *periodic orbit*

Outlook

Can these phenomena be observed in more realistic models?

example:

periodic particle billiards such as Lorentz gas channels



. . .and perhaps even in *experiments*?

(particle in a periodic potential landscape on an annulus?)

References

new results reported in:

G.Knight, O.Georgiou, C.P.Dettmann, R.Klages,
preprint arXiv:1112.3922 (2011)

background literature:

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

(nb: talk and references available on homepage RK)