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Pseudochaos and Stable-Chaos in Statistical Mechanics and Quantum Physics

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Transport in chaotic and non-chaotic systems

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Transport in chaotic and non-chaotic systems

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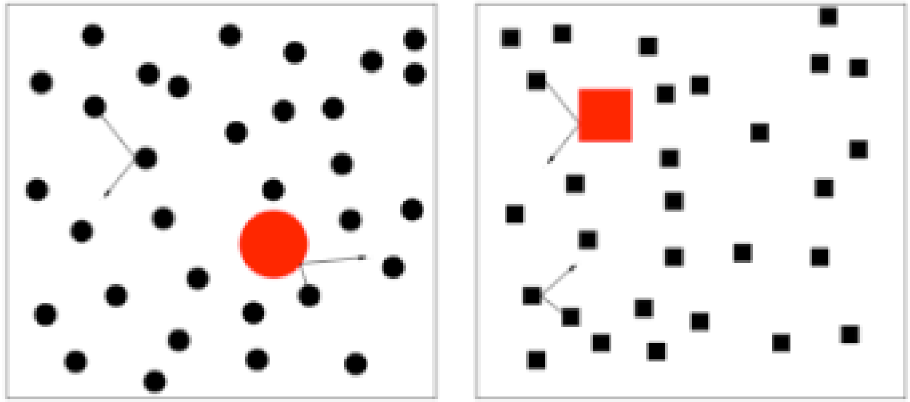


In collaboration with

Fabio Cecconi & Angelo Vulpiani

Transport properties in chaotic and non-chaotic many particle systems
JSTAT: Th.and Exp. P12001 (2007)

General Context

Understanding the role of chaos in statistical mechanics
and, in particular, for the establishment of
good (robust) transport properties

Main goal

Compare -- face to face -- a chaotic and a
non-chaotic many body model able to
generate diffusive motions

Outline

- Motivations through a brief review on the controversial interpretations of an analysis of an experiment on Brownian motion

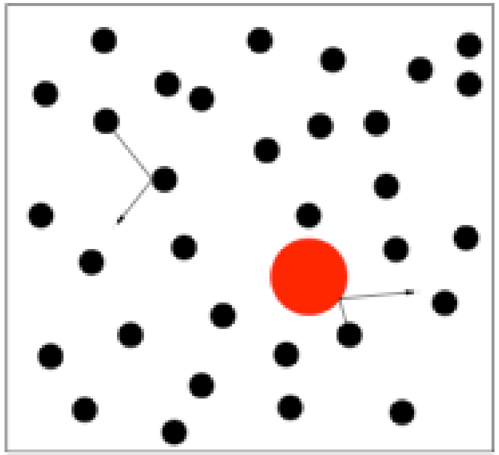
- Introduction of two models for Brownian Motion
  - Chaotic: gas + impurity using hard disks
  - Nonchaotic: gas+impurity using hard parallel squares

- Comparison between the transport & relaxation properties of the two systems

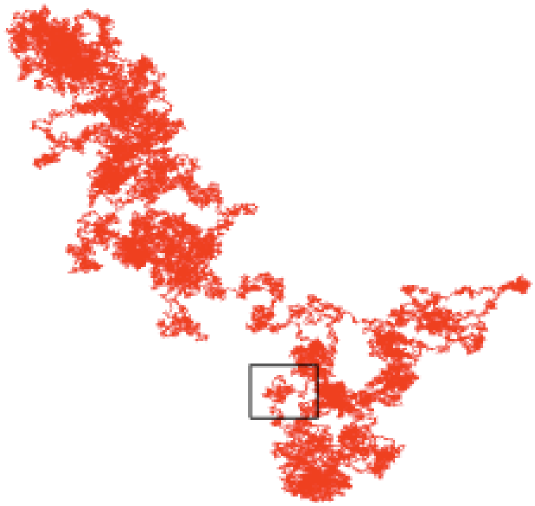
- Some remarks and considerations

Brownian Motion

Pollen (colloid) particles perform BM as a consequence of collisions with molecules of the fluid



$$\langle (x(t) - x(0))^2 \rangle \underset{t\to\infty}{\approx} 2Dt$$



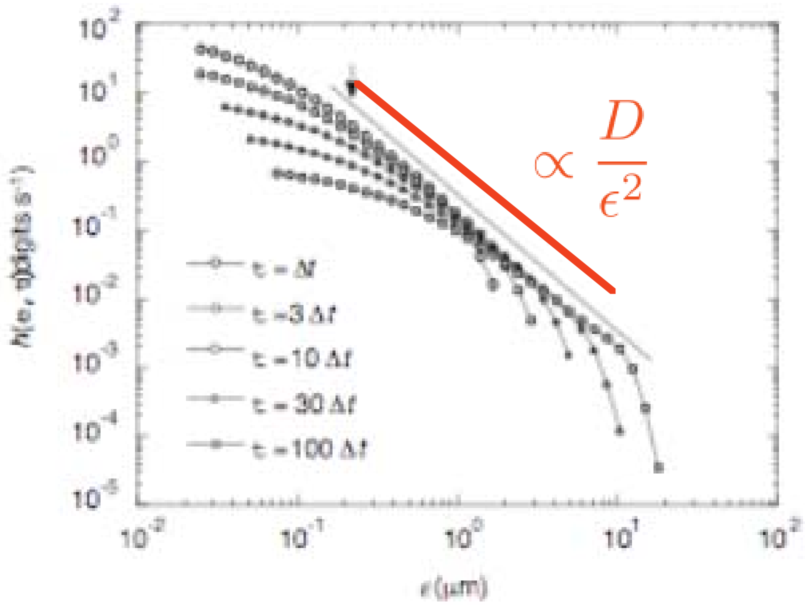
What is the origin of the observed macroscopic diffusive behavior?

Is BM originating from Microscopic chaos?

NATURE | VOL 394 | 27 AUGUST 1998

Experimental evidence for microscopic chaos

P. Gaspard*, M. E. Briggs†, M. K. Francis†, J. V. Sengers†, R. W. Gammon†, J. R. Dorfman† & R. V. Calabrese†

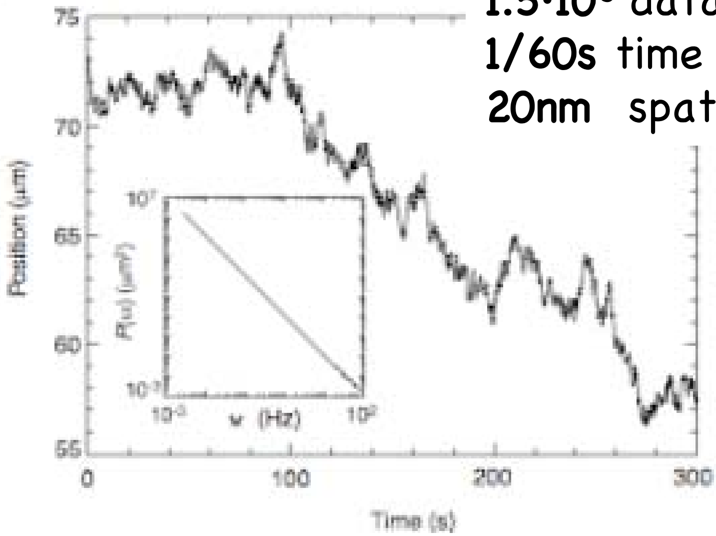


Total time record: **40min**

$1.5 \cdot 10^5$ data points

1/60s time resolution

20nm spatial resolution



$$A\frac{D}{\epsilon^2} \approx h(\epsilon) \leq h_{KS} = \sum_i \lambda_i \Theta(\lambda_i)$$

With the assumption that the System is deterministic we have

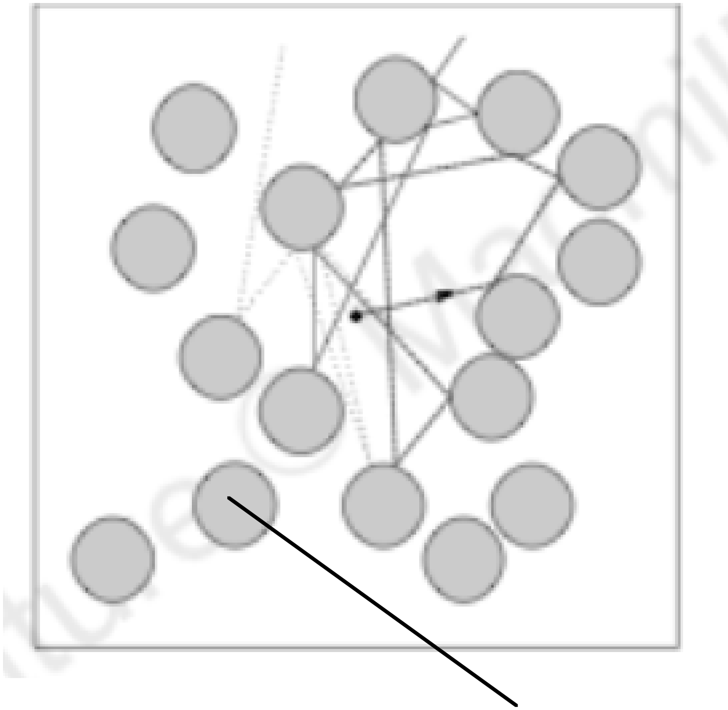
$h_{KS} > 0$ ==> Microscopic Chaos

Basic mechanism

Experimental evidence for microscopic chaos

P. Gaspard[*], M. E. Briggs[†], M. K. Francis[†], J. V. Sengers[†], R. W. Gammon[‡], J. R. Dorfman[‡] & R. V. Calabrese[‡]

Lorentz gas model



Fixed, randomly placed, circular obstacles

BM is thus the result of microscopic Instabilities ensuring memory loss and "randomness" of particle trajectories, at the level of a single particle this can be understood using, e.g., the Lorentz gas

This experiment, its analysis and interpretation raised some debate

Some problem with the interpretation

The raised some criticism which can be summarized as follows

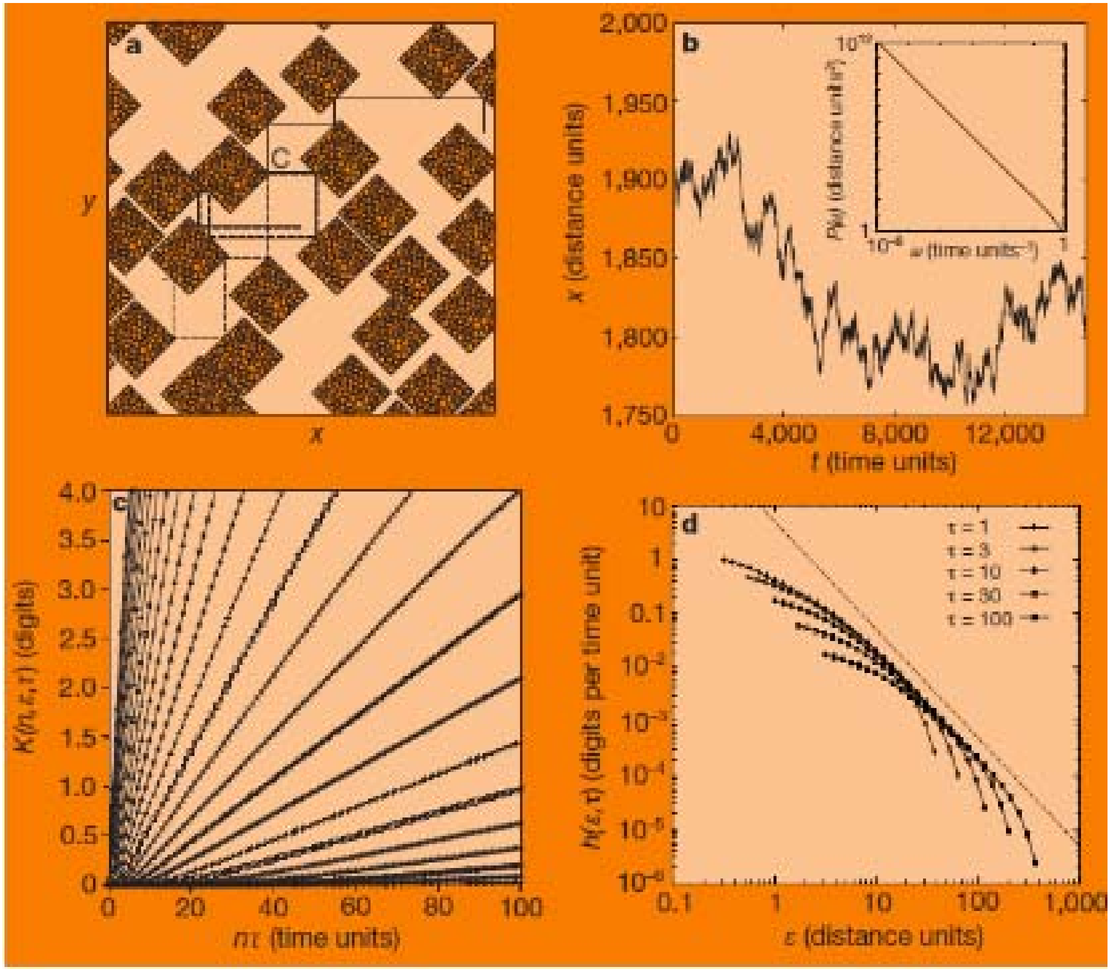
1. Difficulties inherent to the data analysis method. This is in the general longstanding issue of inferring the deterministic (chaotic or regular) or stochastic character of a given system from data analysis only

2. Theoretical difficulties due to the fact that the considered system is infinite dimensional

Problem with finite time and finite resolution

C.P. Dettmann, E.G.D. Cohen & H. van Beijren
Nature (1999)

non-chaotic Ehrenfest wind-tree model



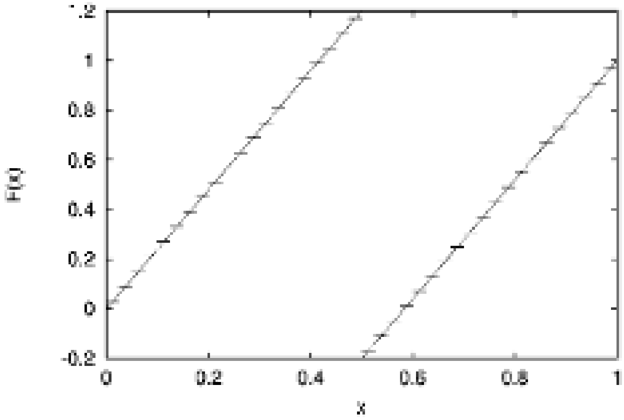
Nonchaotic model: collisions with randomly placed square obstacles

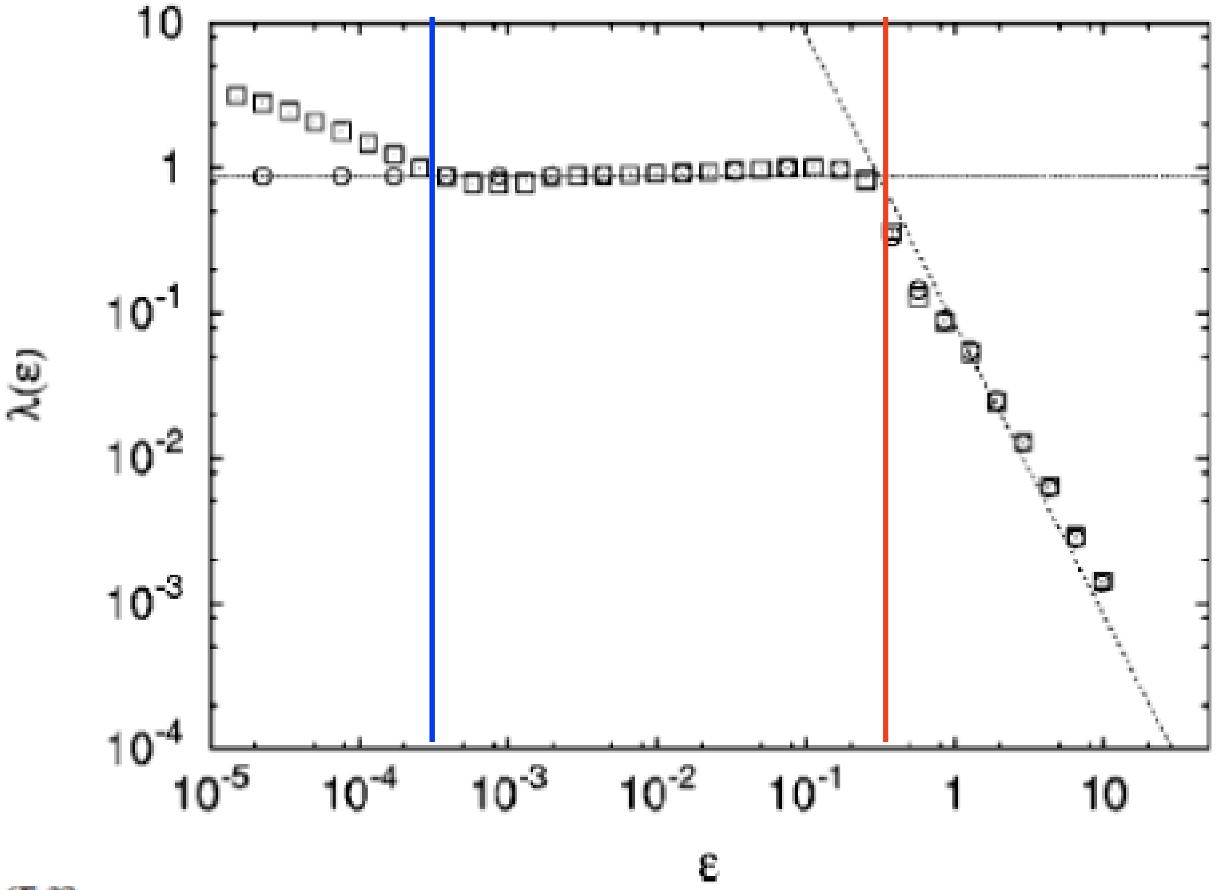
h_{KS}=0 BUT on finite data sequence same features observed in true BM experiment

To detect h_{KS}=0 would require extremely long sequences and fine spatial resolution

Data analysis is inconclusive

Effect of finite resolution





$$x_{t+1} = [x_t] + F(x_t - [x_t]),$$

Chaotic diffusion

$$x_{t+1} = [x_t] + G(x_t - [x_t]) + \sigma \eta_t$$

Chaotic or stochastic? Depends on the observation scale

MC, M. Falcioni, E. Olbrich, H. Kantz & A. Vulpiani PRE (2000)

The problem of the norm & of the exchange of limits

P. Grassberger & T. Schreiber
Nature (1999)

Although the recent literature finds such chaos on a molecular level quite plausible, the observed macroscopic disorder cannot be taken as direct evidence of microscopic chaos. The effectively infinite number of molecules in a fluid can generate the same macroscopic disorder without any intrinsic instability, so brownian motion can be derived for systems that would usually be called non-chaotic, such as a tracer particle in a non-interacting ideal gas. All that is needed for diffusion is 'molecular chaos' in the sense of Boltzmann, that is, the absence of observable correlations in the motion of single molecules.

of freedom. Gaspard *et al.*[1] introduced the term by extrapolating from finite dimensional dynamical systems for which chaos is well defined: on average, initially close states separate exponentially when time tends to infinity. The Lyapunov exponent, or rate of separation, is independent of the particular method used to measure 'closeness'. However, the ideas of diffusion and brownian motion involve infinitely many degrees of freedom. In this thermodynamic limit, Lyapunov exponents are no longer independent of the metric. The large system limit of a finite non-chaotic system will therefore remain non-chaotic with one particular metric and become chaotic with another.

To resolve the confusion, we propose letting the system size tend to infinity first, before the observation time[10]. A system observed in a particular metric μ is then described as μ-chaotic when we find a positive Lyapunov exponent using this metric.

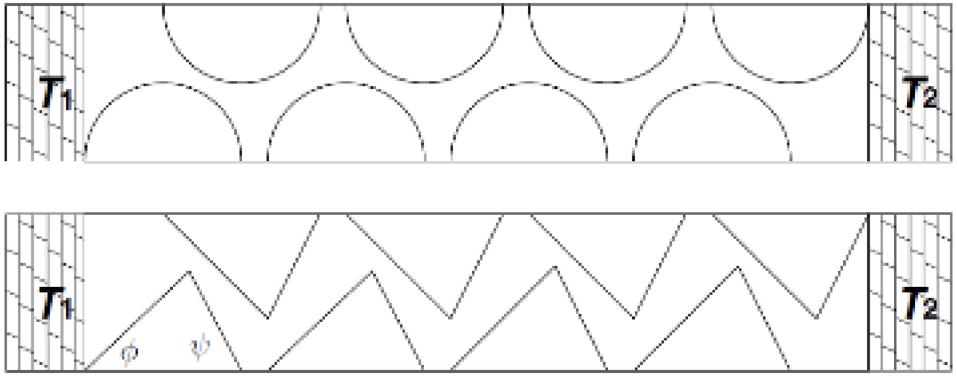
Macroscopic diffusion out of microscopic chaos?

However, this experiment reinvigorated other interesting questions

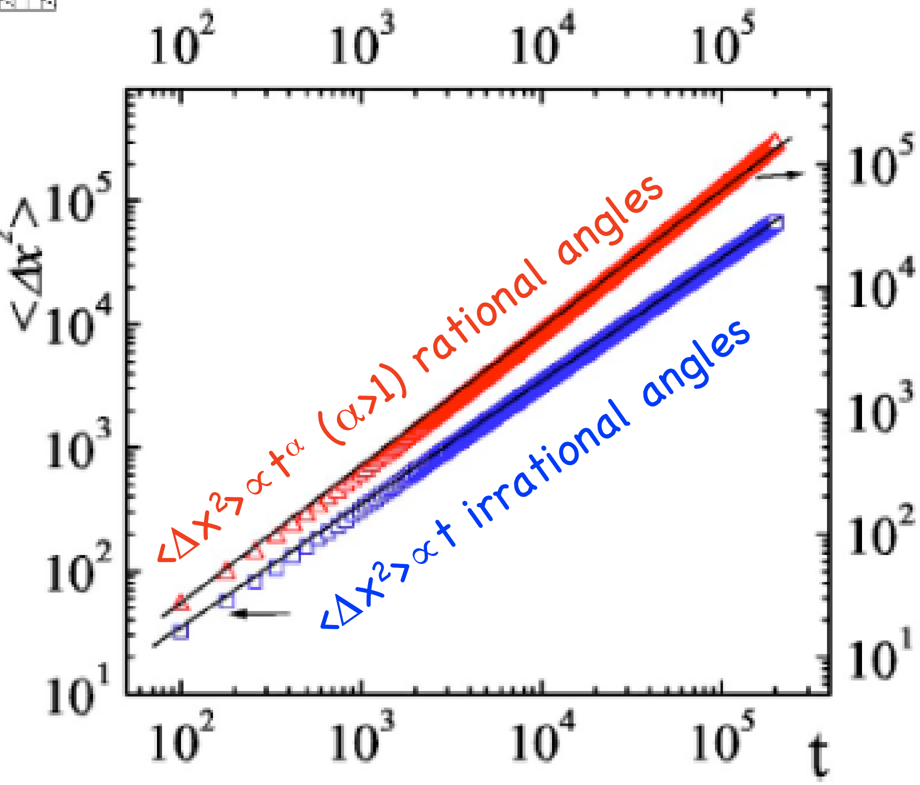
Is chaos a necessary or sufficient condition to macroscopic diffusion and, more in general, for good statistical behaviors?

More in general, what are the requirements for the validity of statistical laws?

Low dimensional examples



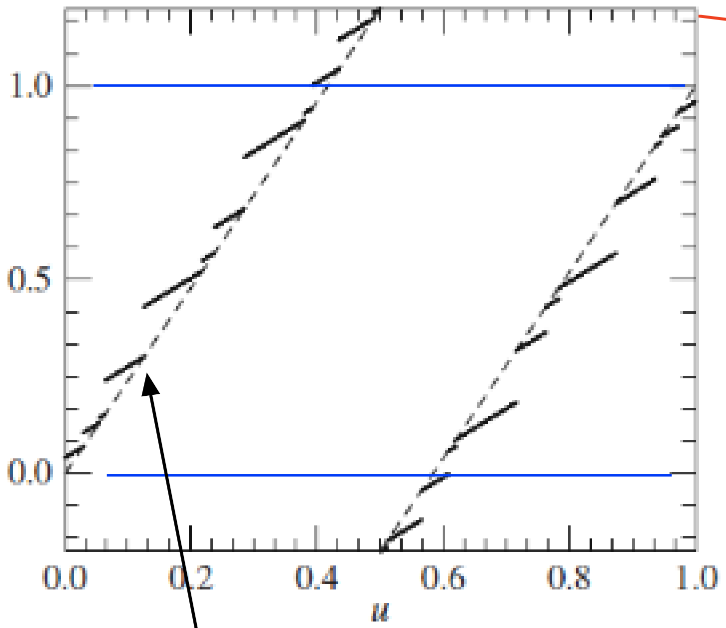
Mass and heat transport are possible also in non-chaotic models



Irrational angles: normal diffusion and validity of Fourier law for heat transport
Rational angles: anomalous diffusion and nonvalidity of Fourier law

Alonso, Artuso, Casati, Guarnieri PRL 1999
Casati & Prosen PRL 2000
Li, Wang & Hu PRL 2002
Li, Casati & Wang PRE 2003

Low dimensional examples

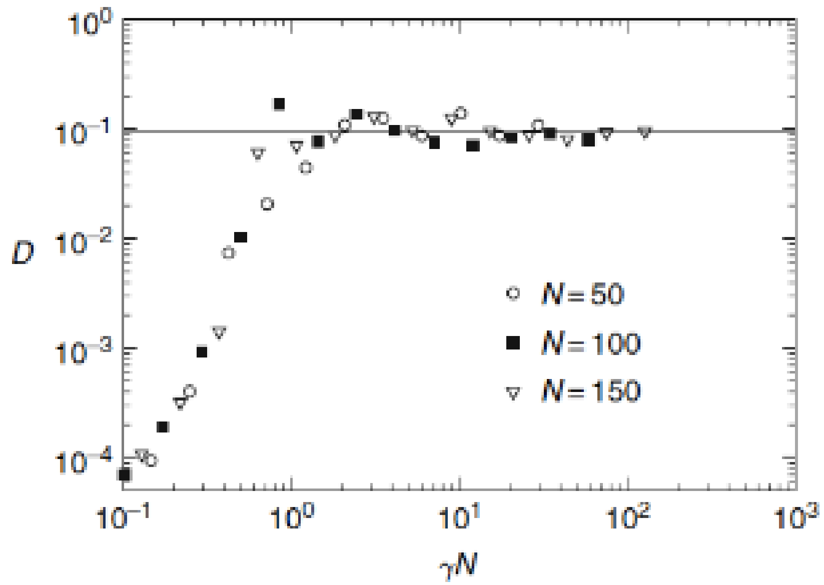


(I) Disorder in their length

$$x(t+1) = [x(t)] + F_\Delta(x(t) - [x(t)]) + \gamma \cos(\alpha t)$$

(II) irrational

Genuine diffusion can be observed
But both (I) and (II) are required

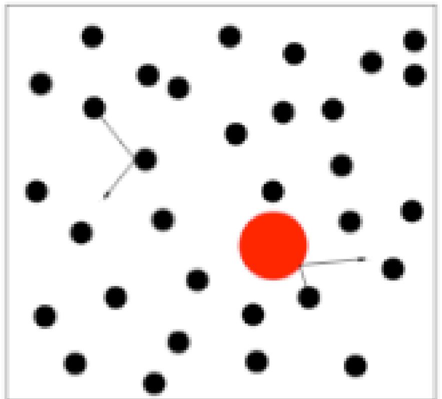


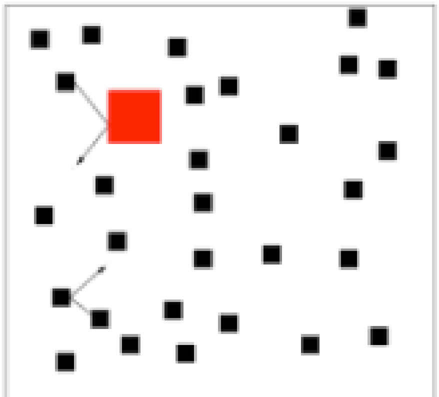
F. Cecconi, D. Del Castillo Negrete,
M. Falcioni & A. Vulpiani Physica D 2003

Two models for BM: gas+impurity

- Low dimensional models are very interesting but in any of them the necessity to avoid periodic orbits requires some mechanisms, making them a bit artificial
- Studying many degrees of freedom systems could provide also some insights on the role of chaos in other statistical aspects
- We will thus consider two many degrees of freedom models for BM

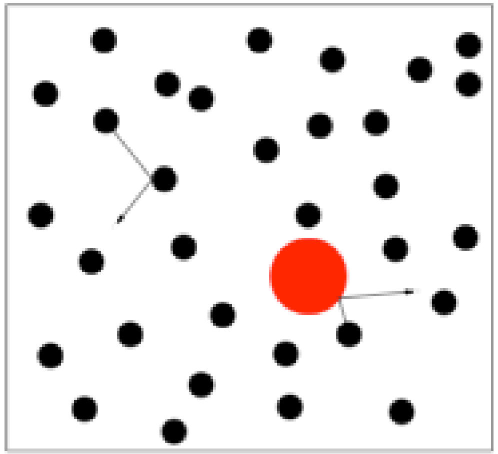
chaotic





nonchaotic

Chaotic model: gas+impurity
[Hard Disks (HD)]



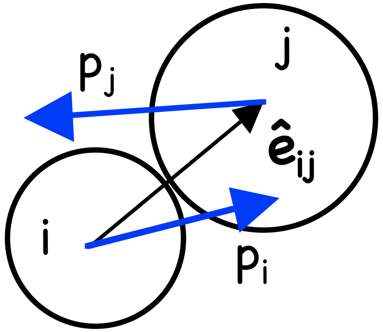
Gas + 1 impurity => N + 1 particles

Free streaming $H = \sum_{j=1}^{N} \frac{\boldsymbol{p}_j^2}{2m} + \frac{\boldsymbol{P}^2}{2M} \equiv \sum_{j=1}^{N+1} \frac{\boldsymbol{p}_j^2}{2m_j}$

+ elastic collisions

$$\boldsymbol{p}_i' = \boldsymbol{p}_i + \frac{2m_i m_j}{m_i + m_j}(\boldsymbol{g}_{ij} \cdot \hat{e}_{ij})\hat{e}_{ij}$$

$$\boldsymbol{p}_j' = \boldsymbol{p}_j - \frac{2m_i m_j}{m_i + m_j}(\boldsymbol{g}_{ij} \cdot \hat{e}_{ij})\hat{e}_{ij}$$

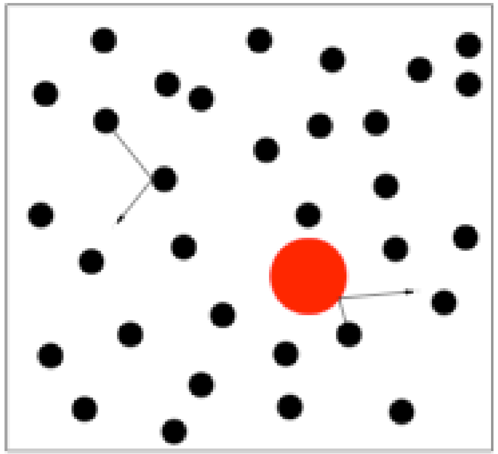


$$\boldsymbol{g}_{ij} = \frac{\boldsymbol{p}_i}{m_i} - \frac{\boldsymbol{p}_j}{m_j} = \boldsymbol{v}_i - \boldsymbol{v}_j$$

Chaos stems from defocusing due to collisions

$$m_i = \begin{cases} m & i = 1, \dots, N \\ M & i = N+1 \end{cases} \qquad (q_i, p_i)_i = \begin{cases} (q_i, p_i) & i = 1, \dots, N \\ (Q, P) & i = N+1 \end{cases}$$

Hard disk model



- well defined statistical mechanics behaviors controlled by energy (temperature), density and volume fraction

$$T = \left\langle \frac{|\boldsymbol{p}_i|^2}{2m} \right\rangle \quad \rho = \frac{N}{L^2} \quad \psi = \frac{N\pi r^2}{L^2}$$

We work in the ψ<<1 limit ($Nr^2 << L^2$) so that the system is akin to a rarefied gas

r, m- gas particle radius & mass
R,M- impurity radius & mass

Two well know limits:

$$\frac{m}{M} \to \infty$$

Lorentz gas (gas->fixed obstacles)

$$\frac{R}{r} \to \infty$$

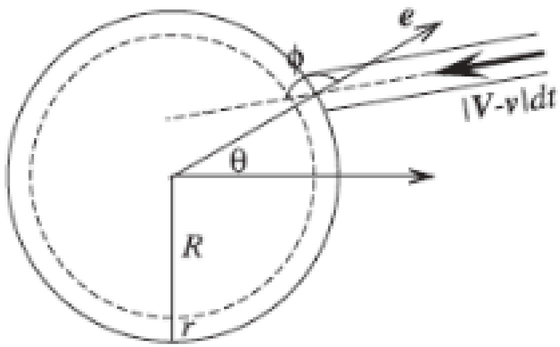
Rayleight-flight (most of collisions involve the impurity)

Transport coefficients in HD

Diffusion of the impurity if M>>m R>>r but still the impurity is a negligible perturbation (this poses constraints at a simulation level)

$$\frac{\mathrm{d}V}{\mathrm{d}t} = -\gamma V + \sqrt{2\gamma \frac{T}{M}}\eta,$$

Effective Langevin equation



$$\left\langle M \frac{\delta \boldsymbol{V}_{\mathrm{n}}}{\delta t} \right\rangle = \frac{2mM}{m+M}\rho(R+r)\int_0^{2\pi}\mathrm{d}\theta \int \mathrm{d}\boldsymbol{v}\, P(\boldsymbol{v})\Theta(-\boldsymbol{e}\cdot\boldsymbol{g})|\boldsymbol{g}\cdot\boldsymbol{e}|(\boldsymbol{g}\cdot\boldsymbol{e})\boldsymbol{e}$$

$$\gamma = 2\sqrt{2\pi}\frac{\rho R\sqrt{mT}}{M}. \qquad C_V(t) = \langle V(t)V(0)\rangle = \langle V^2\rangle e^{-\gamma t} = \frac{T}{M}e^{-\gamma t}$$

Green-Kubo $$D_c = \int_0^\infty C_{VV}(t)dt = \frac{\langle V^2\rangle}{\gamma} = \frac{T}{M\gamma} = \frac{1}{2\sqrt{2\pi}}\frac{1}{\rho R}\sqrt{\frac{T}{m}}$$

Self-diffusion (of a tagged particle)

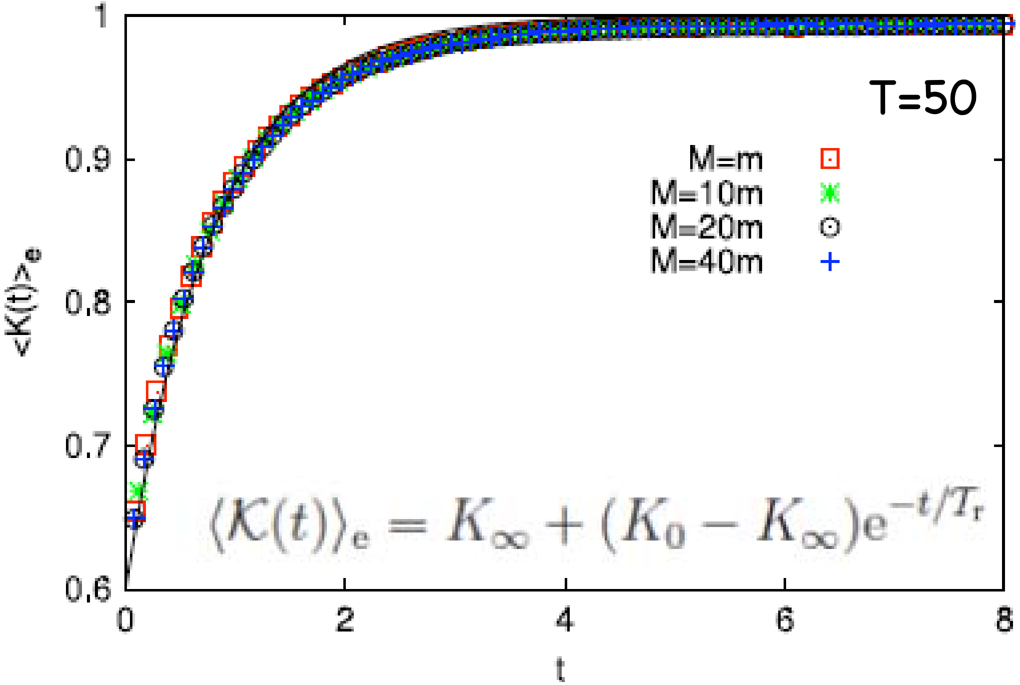
$$D_{\mathrm{g}} = \lim_{t\to\infty}\frac{1}{2t}\langle[x(t)-x(0)]^2\rangle = \frac{1}{4\sqrt{\pi}}\frac{1}{\rho r}\sqrt{\frac{T}{m}}$$

E.g. Dorfman "*An Introduction to chaos in Nonequilibrium Statistical Mechanics* "(CUP 1999))

NB. For self-diffusion no Langevin description (absence of scale separation)
And the formula works only if the impurity does not perturb the gas properties

Some test on HD: relaxation to equilibrium

N=300 & 1000 ρ=10 ψ=O(10^{-3}) R=10r



$$\langle \mathcal{K}(t)\rangle_e = K_\infty + (K_0 - K_\infty)e^{-t/T_r}$$

$$\mathcal{K}(t) = \frac{\overline{v_x(t)^4}}{3\overline{v_x(t)^2}^2} = \frac{\overline{v_y(t)^4}}{3\overline{v_y(t)^2}^2}.$$

$$\overline{v_x^2} = \frac{1}{N}\sum_{i=1}^{N} v_{xi}^2$$

$K_0 = 3/5$

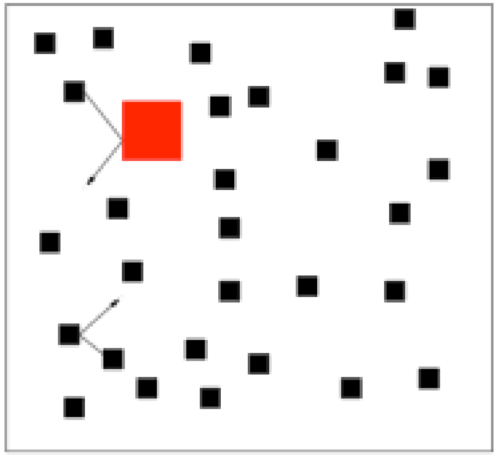
$P_{t=0}(|v|)=1/2v_0$ —t->∞→ $P_{MB}(v)$

The relaxation time is independent of the impurity =>

(1) the impurity is a small perturbation;

(2) relaxation is fast and essentially due to collisions among gas particles

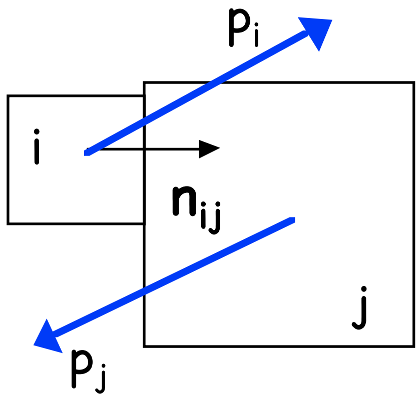
Nonchaotic model: gas+impurity [hard parallel squares (HPS)]



$$\boldsymbol{p}'_i = \boldsymbol{p}_i + \frac{2m_i m_j}{m_i + m_j}(\boldsymbol{g}_{ij}\cdot\hat{\boldsymbol{n}}_{ij})\hat{\boldsymbol{n}}_{ij}$$

$$\boldsymbol{p}'_j = \boldsymbol{p}_j - \frac{2m_i m_j}{m_i + m_j}(\boldsymbol{g}_{ij}\cdot\hat{\boldsymbol{n}}_{ij})\hat{\boldsymbol{n}}_{ij}\,,$$

$$\boldsymbol{g}_{ij} = \frac{\boldsymbol{p}_i}{m_i} - \frac{\boldsymbol{p}_j}{m_j} = \boldsymbol{v}_i - \boldsymbol{v}_j$$



colliding gas particles exchange their velocity components in the impact direction (relabeling)

$$m_1 = m_2 = m \implies v'_1 = v_2 \quad v'_2 = v_1$$

It can be seen as a 2d generalization of 1d hard rods

Some history:
1956 Zwanzig
\`60s Hoover, Adler
\`70s Frisch & co
2009 Hoover & co

Here collisions are not defocusing & chaos is absent

NB. Squares do not rotate, i.e. the system is non-Newtonian

Hard parallel squares

In the absence of impurity, very well characterized as a statistical mechanics model in terms of equation of state, phase transitions etc…

for statistical mechanics very pathological

- particles are independent (no relaxation to equilibrium)
- x,y components do not mix, energy along x and y separately conserved
- non ergodic: infinite number of integral of motions (all velocity moments separately for the velocity components are conserved)
- only marginalization of velocity pdf $P(v_x,v_y) \to P(v_x)P(v_y)$ due to relabeling

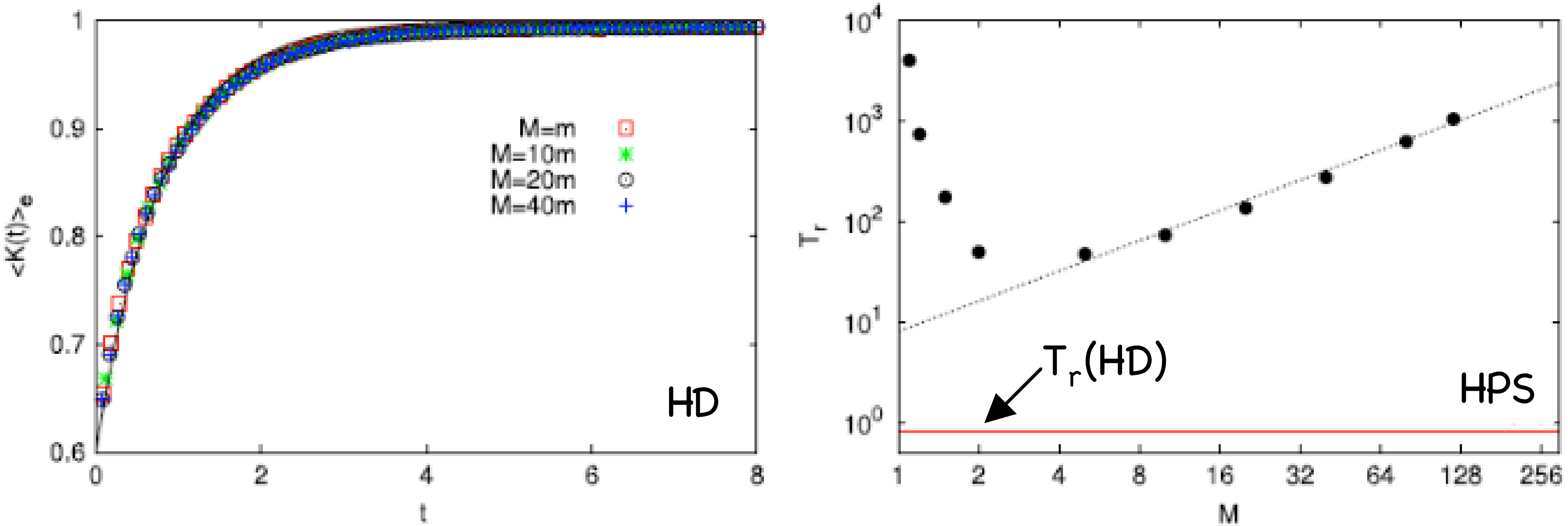
the impurity somehow cures some of the pathologies

- effective coupling among gas particles allowing for energy exchanges during collisions with the impurity ==> equilibrium can be reached (but separately for the two components)

$$P(v_x,v_y) \to P_{MB}(v_x,T_x)P_{MB}(v_y,T_y)$$

Relaxation to equilibrium in HPS

$$\mathcal{K}(t) = \frac{\overline{v_x(t)^4}}{3\overline{v_x(t)^2}^2} = \frac{\overline{v_y(t)^4}}{3\overline{v_y(t)^2}^2}, \qquad \langle \mathcal{K}(t) \rangle_e = K_\infty + (K_0 - K_\infty) e^{-t/T_r}$$

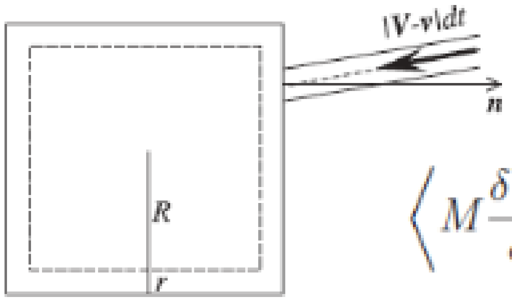


M=m (N+1 equal squares) and M->∞ (fixed obstacle) no relaxation

The relaxation time strongly depends on the mass impurity

Transport coefficients in HPS

Diffusion coefficient of the impurity



$$\frac{dV}{dt} = -\gamma V + \sqrt{2\gamma \frac{T}{M}}\eta;$$

Effective Langevin equation

$$\left\langle M\frac{\delta V_x}{\delta t}\right\rangle \simeq -\frac{4m^2 M}{T(m+M)}\rho(R+r)V_x \sum_{n_x=\pm 1}\int dg_x\, P(g_x)\Theta(-g_x n_x)(g_x n_x)^2|g_x|$$

$$D_c = \frac{\sqrt{\pi}}{8\sqrt{2}}\frac{1}{\rho R}\sqrt{\frac{T}{m}}\left(\frac{1+m/M}{1+r/R}\right)$$

Finite size corrections also
Present in the HD case

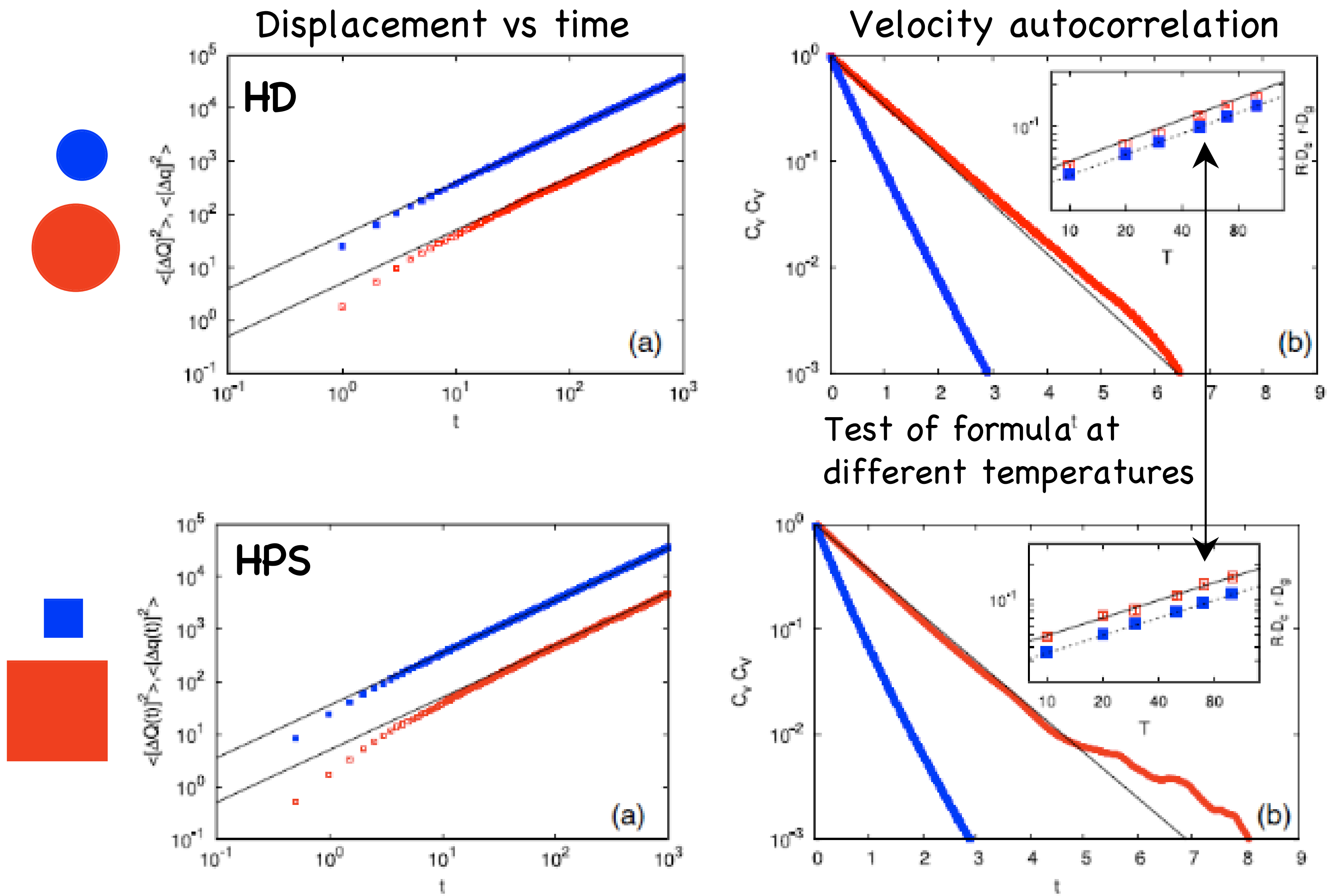
Self diffusion of tagged particles

$$D_g = \frac{\sqrt{\pi}}{16}\frac{1}{\rho r}\sqrt{\frac{T}{m}}.$$

From Szu, Bdzil, Carlier & Frisch PRA 1974

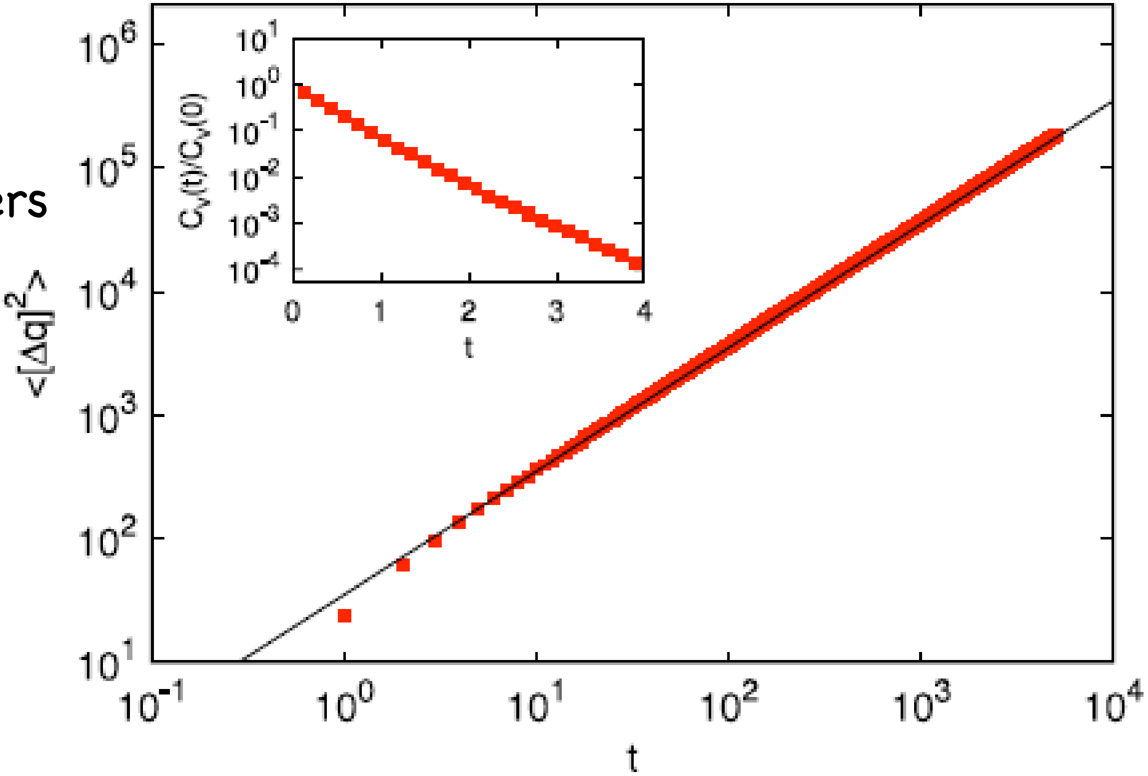
Computed assuming Maxwell-Boltzmann distribution

Impurity diffusion and gas self-diffusion



Self-diffusion without impurity

Same value as with the impurity when holding the same parameters and using MB distribution for velocity

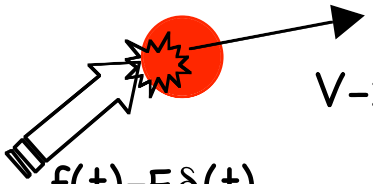


This is an a posteriori consistency test showing that even if the impurity is crucially modifying the statistical mechanics of the system, it is a small perturbation in terms of the transport properties

Relaxation close to equilibrium: FDT

To further test the robustness of the observed transport properties we Also studied the relaxation properties close to equilibrium, i.e. the fluctuation dissipation relation

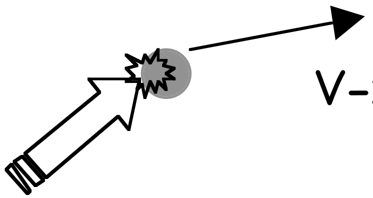
On the impurity $\frac{\mathrm{d}V}{\mathrm{d}t} = -\gamma V + \sqrt{2\gamma \frac{T}{M}}\eta$



V->V+δV_0 If δV_0->0 $$\frac{\langle \delta V(t) \rangle_e}{\delta V_0} = \frac{C_{VV}(t)}{C_{VV}(0)} = e^{-\gamma t}$$

f(t)=Fδ(t)

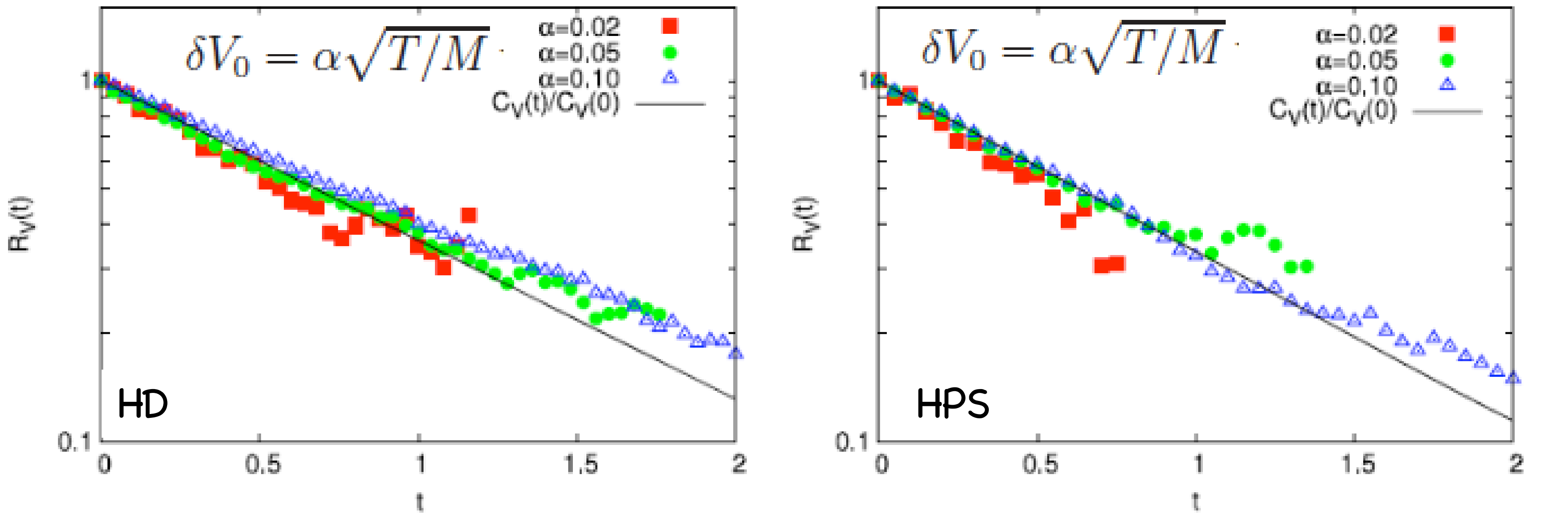
On a gas particle



V->V+δV_0 If δv_0->0 $$\frac{\langle \delta v(t) \rangle_e}{\delta v_0} = \frac{C_{vv}(t)}{C_{vv}(0)}$$

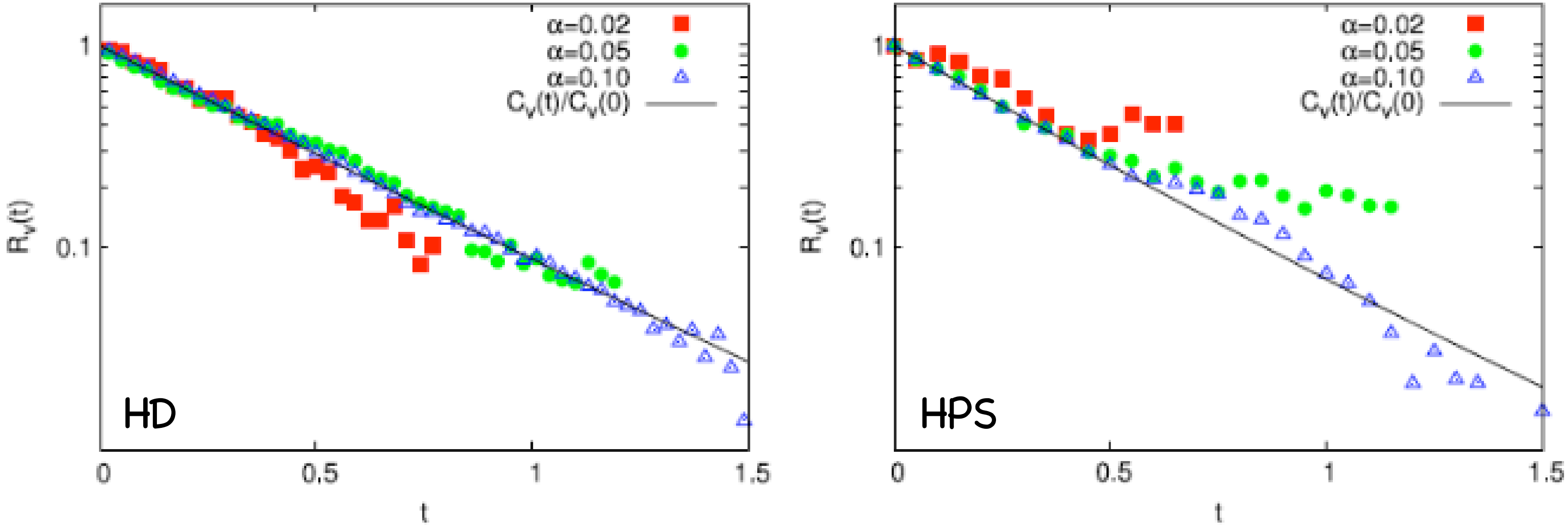
f(t)=Fδ(t)

FDT for the impurity



Provided the perturbation is very small FDT is well satisfied for the impurity

FDT for tagged particles



The same numerical experiment is performed for HD and HPS
in the absence of the impurity.

Note despite the absence of the impurity prevent the HPS from truly relaxing
FDT is fairly well verified, its validity is ensured by the presence of
many degrees of freedom and thus it has a probabilistic origin!

Summary & Conclusions

- Chaos does not seem to be crucial for the validity of robust transport properties (at least from a numerical point of view the chaotic HD and nonchaotic HPS are completely equivalent)

- Also more delicate statistical mechanics properties are very well reproduced in the non-chaotic model with impurity (non-ergodic) and even in the absence of the impurity (non-ergodic & no relaxation)

- The presence of many degrees of freedom seems to be more fundamental in ensuring from a probabilistic point of view what chaos naturally esures at a deterministic level

- We can interpret these results as an extension of Khinchin view (ergodicity is not indispensable to the validity of equilibrium statistical mechanics) to non-equilibrium transport properties

Last remark

HPS with or without impurity is a nice model which can be very useful for testing ideas related to the absence of chaos in a very natural "physical" system.

Thank you!