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**2058-S-14**

**Pseudochaos and Stable-Chaos in Statistical Mechanics and Quantum Physics**

***21 - 25 September 2009***

**Complexity of matter transport in chaotic and non-chaotic particle systems**

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# Complexity of matter transport in chaotic and non-chaotic particle systems

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J. Phys. A 2006, Chaos 2008, Chaos 2009

25 September 2009

http://www.rarenoise.lnl.infn.it/

# Outline

# The problem

Local Thermodynamic Equilibrium, based on separation of scales

$$N \gg 1 \;, \qquad \ell \ll \delta L \ll L \;, \qquad \tau \ll \delta t \ll t$$

$\delta L^3$ contains thermodynamic system $(P, V, T)$;
$\delta t$ suffices for system in $\delta L^3$ to reach equilibrium.

Hydrodynamic laws are given; container shape does **NOT** matter (only boundary conditions): effectively $N, \delta L, L, \delta t, t = \infty$

Differently, in e.g. microporous media, walls and finiteness of space, time and $N$ play significant role to determine transport law: e.g. particle-wall collisions may count more than inter-particle collisions.

Introduce Transport Exponent $\gamma$ as: $\langle \mathbf{r}^2(t) \rangle \sim t^\gamma$

Many studies concerning minimal requirements for $\langle \mathbf{r}^2(t) \rangle \sim t$.
In particular, non-chaotic systems.

Alonso, Artuso, van Beijeren, Casati, Cecconi, Cencini, Cohen, Dettmann, Klages, Larralde, Prosen, Sanders, Swinney, Vulpiani, ...

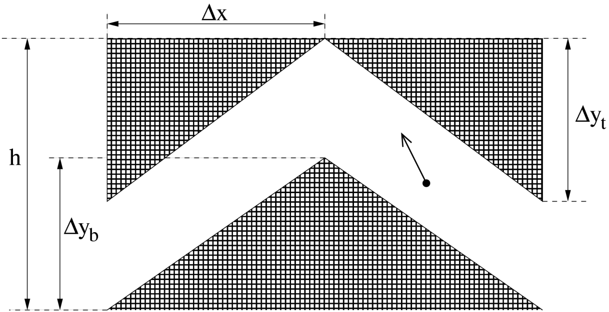
We find that transport is less predictable and affected by all parameters, when LTE does not hold.

Importance of dimensions for correlations decay.

Applications for which asymptotic results are not appropriate (Vulpiani & co.).

# Pointlike particles

If particles don't interact inside polygonal pores, consider them as point-like. Vanishing Lyapunov exp. slow correlation decays. Trajectories slowly separate.




Uniform phase space probability distribution is invariant, but system does not need to be ergodic.

$\gamma$ for parallel walls. 5000 particles, $10^7$ collisions.

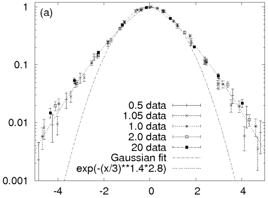
| $\frac{\Delta y}{\Delta x}$ | $h = \Delta y/2$ | $h = \Delta y$ | $h = 1.05\Delta y$ | $h = 2\Delta y$ | $h = 20\Delta y$ |
|---|---|---|---|---|---|
| 0.25 | 1.85 | 1.83 | 1.82 | 1.85 | 1.85 |
| 1 | 1.66 | 1.64 | 1.62 | 1.67 | 1.68 |
| 2 | 1.83 | 1.85 | 1.82 | 1.80 | 1.79 |
| 3 | 1.86 | 1.87 | 1.84 | 1.80 | 1.70 |

For $h \geq 2\Delta y$: infinite horizon.
Error estimated to $\pm 0.03$. Clearly superdiffusive, not ballistic.
Note reduction of $\gamma$ with $h$, for steepest walls.

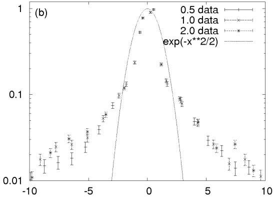
1-flat wall: only longer transients, and even slightly smaller $\gamma$ !

# Very slow decay of correlations.

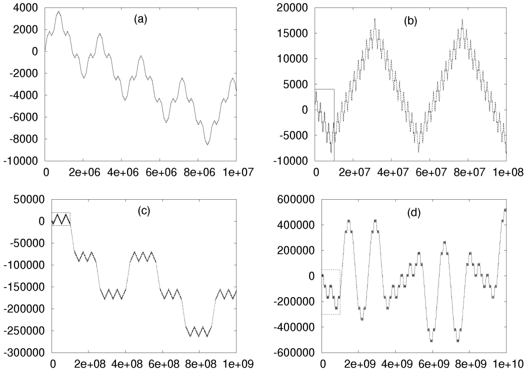
$\Delta y/\Delta x = 2$, i.e. irrational.
Gaussian only close to peak.
Exponential tails. ($10^6$ coll.)




$\Delta y/\Delta x = 1$, i.e. rational.

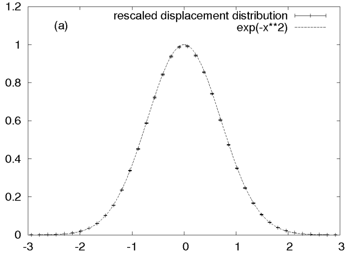



Madness of particle displacement
for $\Delta y/\Delta x = 1$, $d = 2\Delta y$.




Light gas in pore $\sim 1$ nm,
room $T$, $v \sim 400 m/s$, $\tau \sim 1 ps$.
$\Longrightarrow$ correlations over $10^2 \mu s$ and 1 mm.

Unparallel walls. Apparent diffusion.




$\Delta y_t/\Delta x = 0.62$,
$\Delta y_b/\Delta x = 0.65$,
i.e. irrational polygons,
$10^6$ time units ($10^6 - 10^7$ coll.),
$10^4$ initial conditions.

| $\Delta y_t/\Delta x$ | $\Delta y_b/\Delta x$ | $0.5\Delta y$ | $1.0\Delta y$ | $1.05\Delta y$ | $2.0\Delta y$ | $20\Delta y$ |
|---|---|---|---|---|---|---|
| 0.62 | 0.63 | 1.00(2) | 1.02(2) | 0.97(3) | 1.03(7) | 0.72(3) |
| 0.62 | 0.64 | 1.00(1) | 1.2(1) | 1.03(3) | 1.19(7) | 1.10(5) |
| 0.62 | 0.65 | 0.99(2) | 1.02(2) | 1.02(3) | 0.97(6) | 1.13(5) |

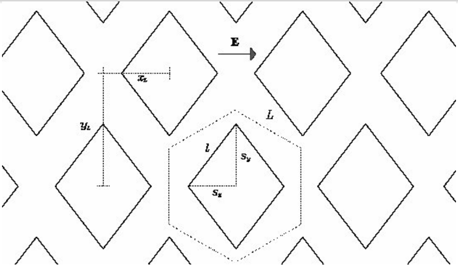
Individual $\approx$ collective behaviour, excpet for rare apparently ballistic trajectories, which may affect collective behaviour.

| $\Delta y_t/\Delta x$ | $\Delta y_b/\Delta x$ | $\gamma$ | $\Delta y_t/\Delta x$ | $\Delta y_b/\Delta x$ | $\gamma$ |
|---|---|---|---|---|---|
| 1 | 1.01 | 0.71(4) | 2 | 2.02 | 1.04(2) |
| 1 | 1.001 | 0.35(6) | 2 | 2.002 | 1.01(2) |
| 1 | 1.0001 | 0.66(5) | 2 | 2.0002 | 1.04(2) |
| 1 | 1.00001 | 0.58(3) | 2 | 2.00002 | 1.02(2) |
| 1 | 1.000001 | 0.53(5) | 2 | 2.000002 | 0.98(2) |
| 1 | 1 | 1.66(3) | 2 | 2 | 1.83(3) |

Apparently, no trend towards super-diffusion, close to (rational or irrational) parallel cases, for **fixed simulation times**.
Sanders-Larralde irrational case: crossover time from anomalous to normal diverges as walls turn parallel. **But membrane is finite!**
Macroscopically less predictable,
though microscopically more stable than chaotic systems;
sensitive dependence of transport on geometry:
not just transport coefficient but transport law looks highly irregular in **finite membranes**.

# Nonequilibrium Eherenfest Gas (L.R.B. JSP 2000)

Field focuses trajectories; non-defocussing scatterers, but non-linearities (jumps and free flights).

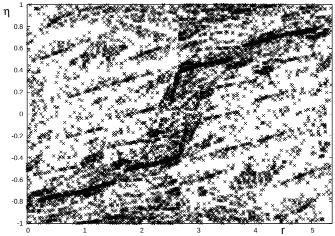


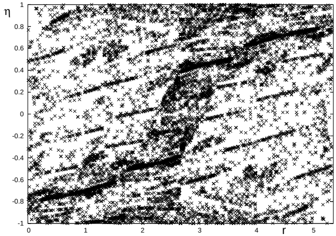

$$\begin{cases} \dot{x} = p_x/M \ , & \dot{p}_x = \epsilon - \alpha(\mathbf{p})p_x \\ \dot{y} = p_y/M \ , & \dot{p}_y = -\alpha(\mathbf{p})p_y \end{cases} \quad \text{with} \quad \alpha(\mathbf{p}) = -\epsilon p_x$$

| Field | Collisions | Lyapunov exponent |
|---|---|---|
| 0.374 | $10^6$ | 0.144232 |
| 0.374 | $1.5 \times 10^7$ | 0.144317 |
| 0.374 | $6.5 \times 10^7$ | 0.144291 |
| 0.374 | $2.15 \times 10^8$ | 0.144320 |
| 0.5 | $5 \times 10^7$ | 0.166648 |
| 0.5 | $2 \times 10^8$ | 0.166622 |

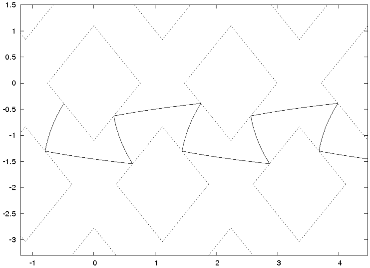
Large fields (high dissipation and focussing power) yet positive Lyapunov apparently quite well resolved

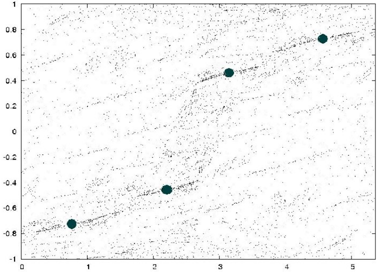
## “Attractor” after 5 $10^7$ and 1.8 $10^8$ collisions



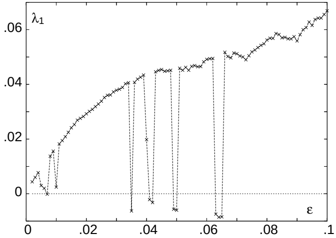



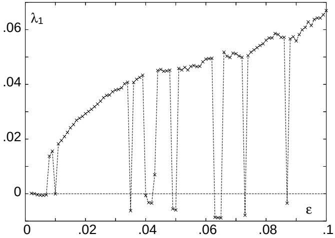

## Embedded, unstable periodic orbit ($\lambda_1 = 0.108... > 0!$)



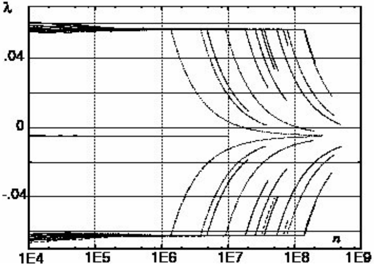



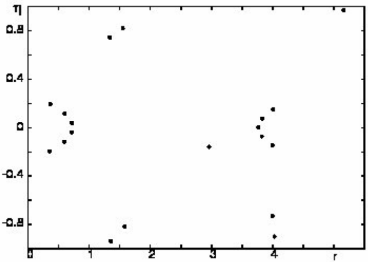
# "Lyapunov" after $10^7$ and $3\ 10^8$ collisions




# Collapse onto attracting periodic orbit



After $O(10^8)$ collisions, most apparently weakly chaotic states survive, despite high dissipation: chaos quite plausible, but cannot exclude collapse on periodic orbits after much longer times.

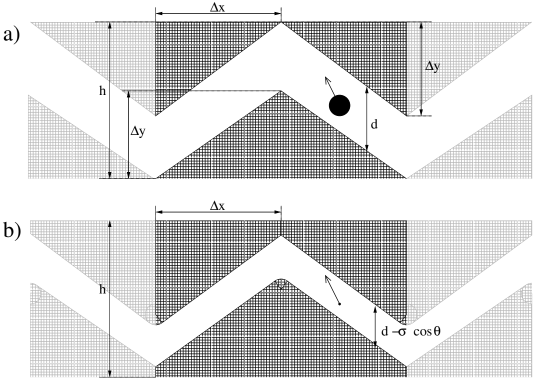
No purpose to continue. It suffices to note peculiar behaviour over very long times:

- abrupt transition from low-period attractors to apparently chaotic steady states; current jumps (discontinuous? Variations of less than $10^{-5}$).
- periodic attractors always seem to coexist with transiently chaotic states.

Same phenomenology if rhombus angles are varied.

# Finite Size Particles

Anomalous point-like diffusion: $\Delta y/\Delta x = 1$ or 2. $\sigma =$ particle diameter.




Semidispersive billiard with bumps ergodicity not known. Collisions with rounded corners and interactions may lead to positive Lyapunov exponents.

$$D_s(N;t) = \sum_{i=1}^{N} \int_0^t \frac{\langle \mathbf{v}_i(0)\mathbf{v}_i(s)\rangle}{2dN} ds \;, \quad D_0(N;t) = \sum_{i,j=1}^{N} \int_0^t \frac{\langle \mathbf{v}_i(0)\mathbf{v}_j(s)\rangle}{2dN} ds$$

Let $f_{\text{apex}}$ = apex collision frequency;
$\tau_{\text{apex}}$ = mean apex collision time.
Initially: point-like transport in pores of reduced height;
super-diffusive, $\gamma$ determined by wall angle.

Departure to **apparently** reach diffusive behaviour at O(10) $\tau_{\text{apex}}$.

Departure points overlap if time rescaled by $t' = tf_{\text{apex}}$.

However, convergence to diffusive behaviour remains not obvious.
Even if departure from pointlike case occurs after 10 $\tau_{\text{apex}}$,
$10^3\tau_{\text{apex}}$ and averaging over $10^5$ initial conditions are not sufficient.

Averages over two different sets of $10^5$ initial conditions **still differ**.

Unpredictable.

Interparticle collisions introduce further randomizing, decorrelating, mechanisms: defocussing collisions occur at random positions (hence impair the "bursts").

Departure from polygonal billiard phase takes place on the shortest time scale between $1/f_{\rm apex}$ and $1/f_{\rm coll}$.

Convergence to diffusion, now common, is determined by $f_{\rm coll}$.

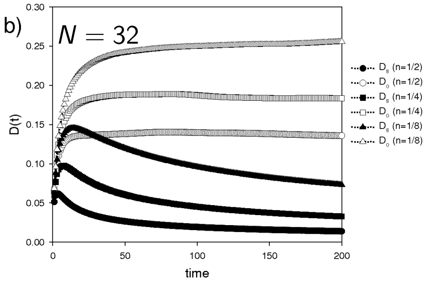
However, for $N \leq 10$, kinetic theory prediction

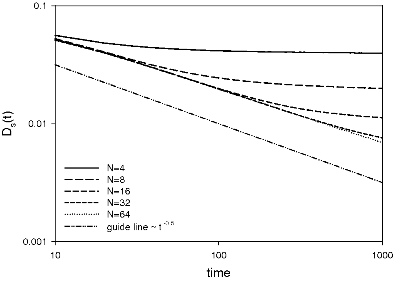
$$D_s^{(\text{2D-Enskog})} = \frac{1}{2n\sigma g(\nu)}\sqrt{\frac{kT}{\pi m}} \; ; \quad g(\nu) = \frac{1-7\nu}{16(1-\nu)^2} \; ; \quad \nu = \frac{\pi n \sigma^2}{4}$$

and even simply $1/n$ behaviour are not verified (unpredictable).

Convergence rather quick ($N \geq 16$)

Single File Transport ($\sigma > d/2$, cannot overtake); some correlation persists (particles order). Kinetc theory: $\gamma = 1/2$, for $N \to \infty$.
Stable phenomenon due to low dimensionality.




Finite $N$, $D_s$ only reduced, but $\gamma \to 1/2$ as $N \to \infty$;
$D_0$ differs from $D_s$ values: order correlations persist.

Here, $f_{apex} \sim f_{coll}$: more efficient interparticle collisions.
$D_s \to D_0$ if $\sigma \to 0$, not if $n \to 0$ **(importance of interactions).**

# Take home message

**Definition.** Parameters $y \in I$ (interval width $h$), $t_{\mathrm{MAX}} \in (0, \infty)$.
Transport law: $\langle s_x^2(t) \rangle \approx A t^\gamma$, $t \in [0, t_{\mathrm{MAX}}]$ (e.g. least squares).
$\Delta\gamma(y_m, y_M) =$ largest $\gamma$-variation for $y \in (y_m, y_M) \subset I$.

**i.** *$t_{\mathrm{MAX}}$-transport complexity of first kind in $(y_m, y_M)$:*

$$\mathcal{C}_1(y_m, y_M) = \frac{h \Delta\gamma(y_m, y_M)}{2(y_M - y_m)}$$

**ii.** *$t_{\mathrm{MAX}}$-transport complexity of second kind for $y = \hat{y}$: $\mathcal{C}_2(\hat{y})$ such that*

$$\lim_{\varepsilon \longrightarrow 0} \frac{\mathcal{C}_1(\hat{y} - \varepsilon, \hat{y} + \varepsilon)}{\varepsilon^{\mathcal{C}_2(\hat{y})}} < \infty$$

**iii.** *$t_{\mathrm{MAX}}$-transport complexity of third kind for $y = \hat{y}$:*

$$\mathcal{C}_3(\hat{y}) = \lim_{\varepsilon \longrightarrow 0} \Delta\gamma(\hat{y} - \varepsilon, \hat{y} + \varepsilon)$$

- Point particles are peculiar, but finite-sized particles behave similarly within given **finite** space and time scales.
  Can be diffusive (chaos not necessary), but highly irregular.
- $N \geq 2$: diffusion sets in even if $f_{\text{coll}} \ll f_{\text{apex}}$; interactions randomness counts more than chaos for normal transport (faster **correlations** decay), CCV-07, LMP-09.
- Single file: sub-diffusive for $N \to \infty$; low dimensionality preserves certain **correlations** (chaos not sufficient).
- Geometry effects and **correlations** lasting over scales comparable with medium size, more interesting than asymptotics: e.g. relevance for nano- bio-sciences.
- Macroscopic un-predictability (sensitive dependence)
- **N≫1, 3 dimensions, particle collisions**

# References


- JEPPS O G, RONDONI L. (2006). Thermodynamics and complexity of simple transport phenomena. JOURNAL OF PHYSICS. A, MATHEMATICAL AND GENERAL, vol. A 39; p. 1311-1338, ISSN: 0305-4470
- O. G. JEPPS, C. BIANCA, RONDONI L. (2008). ONSET OF DIFFUSIVE BEHAVIOUR IN CONFINED TRANSPORT SYSTEMS. CHAOS, vol. 18; p. 013127-1-013127-13, ISSN: 1054-1500
- C. BIANCA, RONDONI L. (2009). The nonequilibrium Ehrenfest gas: a chaotic model with flat obstacles?. CHAOS, vol. 19; p. 013121-1-013121-10, ISSN: 1054-1500