

Institut Non Linéaire de Nice

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Fractality of the Hydrodynamic Modes of Diffusion

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Overview

Paradigm : The classical dynamics of systems of large numbers of particles is typically chaotic.



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Low-dimensional model systems can be used to obtain *quantitative information on non-equilibrium processes in terms of the chaotic properties of the dynamics.*





Overview

Paradigm : The classical dynamics of systems of large numbers of particles is typically chaotic.

Low-dimensional model systems can be used to obtain *quantitative information on non-equilibrium processes in terms of the chaotic properties of the dynamics.*

The result consists in a collection of **dimension formulae** relating transport coefficients to the characteristic quantities of chaos, as well as an **entropy production formula.**



Gaussian Thermostatted Systems

E.G.D. Cohen, C.P. Dettmann, D. Evans, W.G. Hoover, G.P. Morriss, H.A. Posch



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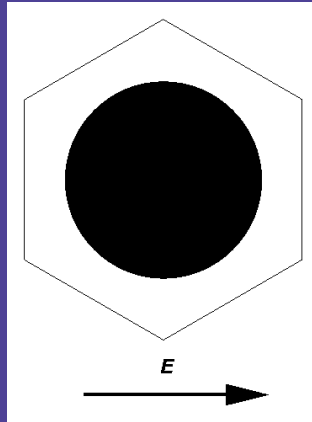
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Gaussian Thermostatted Systems

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Example : the thermostatted field-driven Lorentz gas



- Elastic collisions : $\mathbf{p} \rightarrow \mathbf{p}' = \mathbf{p} - 2(\mathbf{p} \cdot \hat{\mathbf{k}})\hat{\mathbf{k}}, p'^2 = p^2;$
- Between collisions : $\dot{\mathbf{p}} = q\mathbf{E} - \alpha\mathbf{p};$
- Gaussian thermostating : $p^2 = \text{const.} \Rightarrow \alpha = q\mathbf{E} \cdot \mathbf{p}/p^2.$



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This system has *phase space contraction*

$$\partial_{\mathbf{r}}\dot{\mathbf{r}} + \partial_{\mathbf{p}}\dot{\mathbf{p}} = -\alpha$$

The stationary state is fractal :

$$\lambda_+ + \lambda_- = -\langle\alpha\rangle < 0$$



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The entropy production rate is

$$\frac{\mathbf{J} \cdot \mathbf{E}}{T} = \sigma \frac{E^2}{T} = k_B \langle\alpha\rangle = -k_B(\lambda_+ + \lambda_-)$$



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We infer the expression of the *electrical conductivity*

$$\sigma = -\frac{k_B T}{E^2}(\lambda_+ + \lambda_-)$$



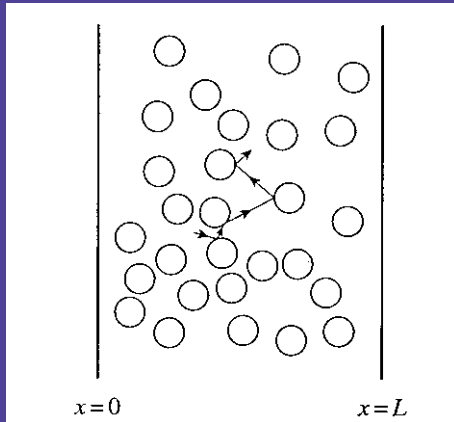
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Escape Rate Formalism

F. Baras, J. R. Dorfman, P. Gaspard, G. Nicolis

Example : the Lorentz gas on an open slab



- Volume-preserving dynamics;
- Absorbing boundary conditions.



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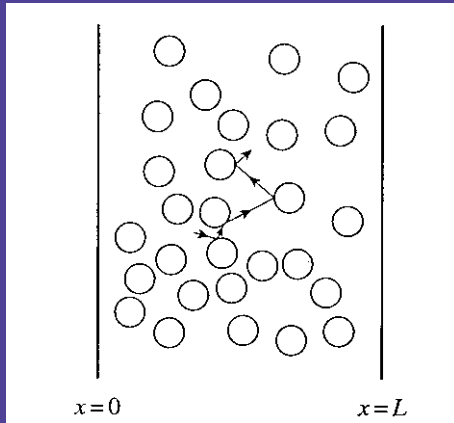
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Escape Rate Formalism

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Example : the Lorentz gas on an open slab



- Volume-preserving dynamics;
- Absorbing boundary conditions.

This system satisfies a diffusion equation $\partial_t \rho = \mathcal{D} \partial_x^2 \rho$ which describes the evolution of a *macroscopic density* ρ with *decay rate*

$$\gamma_{\text{macro}} = \frac{\pi^2}{L^2} D$$



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At the level of the dynamics, almost every trajectory will escape. However, there is an uncountable number of trapped trajectories which define a fractal repeller .



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The repeller is an *invariant measure* which is not smooth and such that

$$\begin{aligned}\lambda_+ &\neq h_{KS}, & \gamma_{\text{micro}} &\equiv \lambda_+ - h_{KS} \\ \lambda_+ &= -\lambda_-\end{aligned}$$



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The identification of the macro- and microscopic escape rates yields the relation

$$\mathcal{D} = \lim_{L \rightarrow \infty} \left(\frac{L}{\pi} \right)^2 \begin{cases} (\lambda_+ - h_{KS}) \\ \lambda_{+C_I} \\ \lambda_{+C_H} \end{cases}$$



Hydrodynamics (simple)

For the diffusion equation

$$\partial_t \rho = \mathcal{D} \nabla^2 \rho$$

the hydrodynamic modes are the solutions of the form

$$\rho_{\mathbf{k}}(\mathbf{r}, t) = \exp(s_{\mathbf{k}} t) \exp(i\mathbf{k} \cdot \mathbf{r})$$



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The modern theory of dynamical systems offers the appropriate tools to define these modes in the context of deterministic systems.



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Hydrodynamic modes from Liouvillian Dynamics

We assume quasi-periodic boundary conditions :

- periodicity of the *dynamics* over the configuration space;
- do not impose periodicity of the *probability density* (global normalization).



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Hydrodynamic modes from Liouvillian Dynamics

We assume quasi-periodic boundary conditions :

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- do not impose periodicity of the *probability density* (global normalization).

The non-periodic probability density can be decomposed into its Fourier modes.



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Tagged Particle Diffusion

- the wavenumber of the Fourier mode of the probability density is identical to \mathbf{k} of the hydrodynamic mode;



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Tagged Particle Diffusion

- the wavenumber of the Fourier mode of the probability density is identical to \mathbf{k} of the hydrodynamic mode;
- $s_{\mathbf{k}}$ from the dispersion relation is then identified to a [Pollicott-Ruelle resonance](#) ;



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Tagged Particle Diffusion

- the wavenumber of the Fourier mode of the probability density is identical to \mathbf{k} of the hydrodynamic mode;
- $s_{\mathbf{k}}$ from the dispersion relation is then identified to a [Pollicott-Ruelle resonance](#) ;
- The corresponding eigenstate is a [hydrodynamic mode of diffusion](#).



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Multibaker Map

Consider a collection of cells consisting of unit squares, indexed by an integer $n = 1, \dots, L$.





Multibaker Map

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The dynamics is a time-discretized process defined by the 3-adic map:

$$B : (n, x, y) \rightarrow \begin{cases} (n - 1, 3x, y/3), & 0 \leq x < 1/3 \\ (n, 3x - 1, (y + 1)/3), & 1/3 \leq x < 2/3 \\ (n + 1, 3x - 2, (y + 2)/3), & 2/3 \leq x < 1 \end{cases}$$

(assume globally periodic boundary conditions : $n = 1$ is identified with $L + 1$)



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Note: the volumes are preserved and the dynamics is time-reversible.



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Liouvillian Dynamics

Probability densities $g_\tau(n, x, y)$ are evolved by the Perron-Frobenius operator.



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Let $W_\tau(n) = \int_0^1 dx dy g_\tau(n, x, y)$. This is the equivalent of a macroscopic density. It is evolved according to

$$W_{\tau+1}(n) = \frac{1}{3}W_\tau(n+1) + \frac{1}{3}W_\tau(n) + \frac{1}{3}W_\tau(n-1)$$





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which is analogous to a random walk with diffusion coefficient $\mathcal{D} = 1/3$: in the continuum limit ($\tau \rightarrow t, n \rightarrow x$) it reduces to

$$\partial_t w(t, x) = \frac{1}{3} \partial_x^2 w(t, x)$$





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The eigenmodes of the discrete equation are $\psi_k(n) = \exp(ikn)$, with eigenvalues $\chi_k = 1/3[1 + 2 \cos(k)]$, $k = 2\pi m/L$ ($m = 0, \dots, L-1$).





Cumulative measures

Let

$$G_{\tau}(n, y) = \int_0^1 dx \int_0^y dy' g_{\tau}(n, x, y')$$



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$$G_\tau(n, y) = \int_0^1 dx \int_0^y dy' g_\tau(n, x, y')$$

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$$G_\tau(n, y) = \sum_k a_k (\chi_k)^\dagger \psi_k(n) F_k(y)$$



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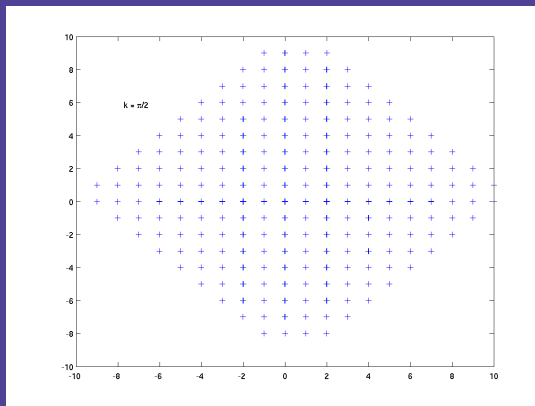
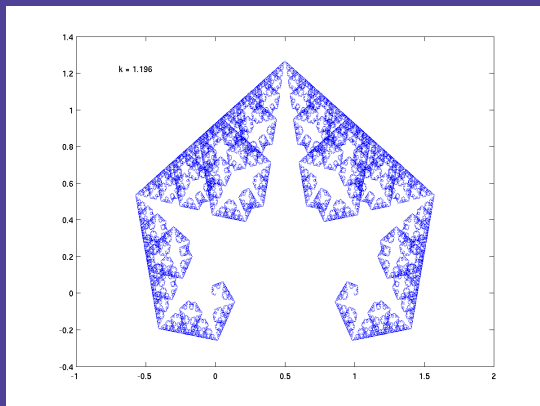
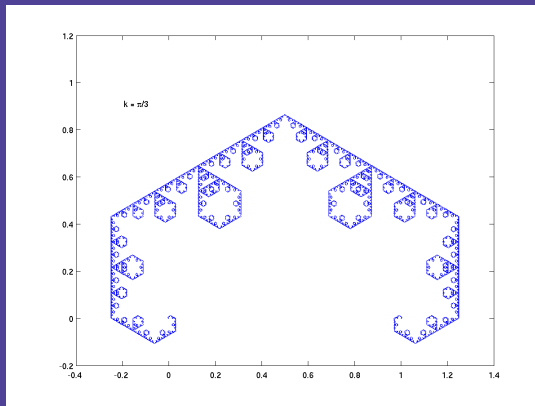
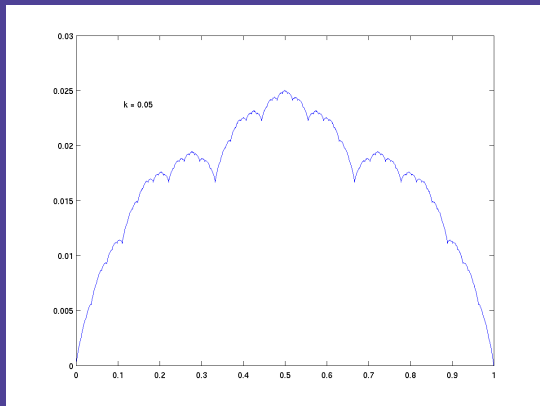
The modes F_k are solutions of a de Rham functional equation :

$$F_k(y) = \begin{cases} \frac{\exp(ik)}{3\chi_k} F_k(3y), & 0 \leq y < 1/3 \\ \frac{1}{3\chi_k} F_k(3y - 1) + \frac{\exp(ik)}{3\chi_k} F_k(1), & 1/3 \leq y < 2/3 \\ \frac{\exp(-ik)}{3\chi_k} F_k(3y - 2) + \frac{1 + \exp(ik)}{3\chi_k} F_k(1), & 2/3 \leq y < 1 \end{cases}$$



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Fractal Dimension

If $|k|$ is not too large, we can compute the Hausdorff measure associated to cylinder sets of width $1/3^l$:

$$\Gamma_l^d(F_k) = \sum_{\omega_1, \dots, \omega_l} |\Delta F_k[y(\omega_1, \dots, \omega_l)]|^d$$

The Hausdorff dimension of F_k is defined as $D_H(k)$ such that

$$\lim_{l \rightarrow \infty} \Gamma_l^d(F_k) = \begin{cases} \infty, & d < D_H(k) \\ 0, & d > D_H(k) \end{cases}$$

The solution is

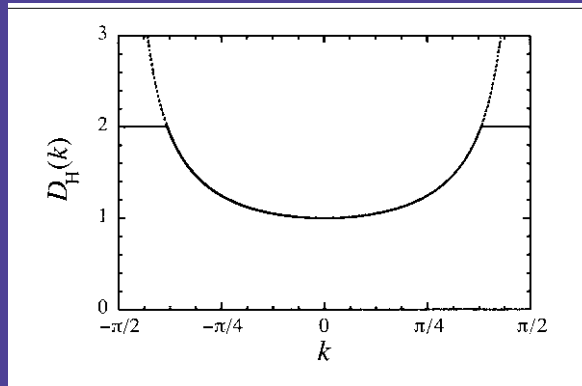
$$D_H(k) = \begin{cases} \log(3)/\log(3\chi_k), & |k| < k_f \\ 2, & k_f \leq |k| < k_c \end{cases}$$



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Dimension Formula

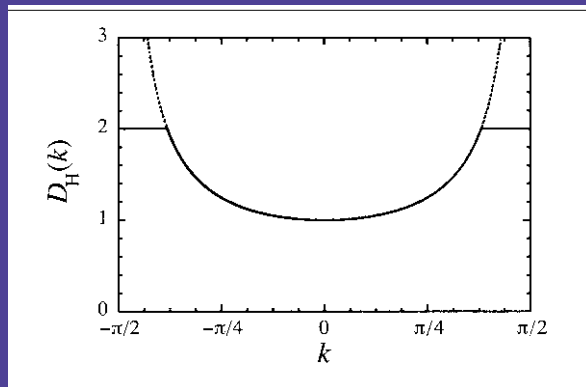


The cumulative function of the hydrodynamic mode of wavenumber k has Hausdorff dimension

$$D_H(k) = 1 + \frac{\mathcal{D}}{\lambda_+} k^2 + \mathcal{O}(k^4)$$



Dimension Formula



The cumulative function of the hydrodynamic mode of wavenumber k has Hausdorff dimension

$$D_H(k) = 1 + \frac{\mathcal{D}}{\lambda_+} k^2 + \mathcal{O}(k^4)$$

Conversely,

$$\mathcal{D} = \lim_{k \rightarrow 0} \frac{1}{k^2} \lambda_+ [D_H(k) - 1]$$





Lorentz gases

The dimension formula extends to all chaotic systems with 2 degrees of freedom. For Lorentz gases, one considers the decay rate of the *Van Hove intermediate incoherent scattering function* as

$$s_{\mathbf{k}} = \lim_{t \rightarrow \infty} \frac{1}{t} \log \langle \exp\{i\mathbf{k} \cdot [\mathbf{r}_t - \mathbf{r}_0]\} \rangle$$

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Lorentz gases

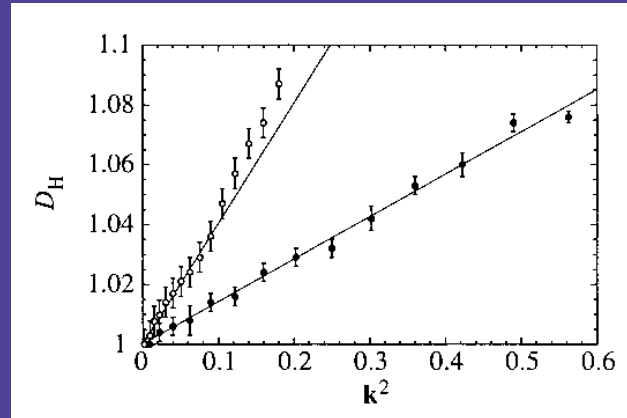
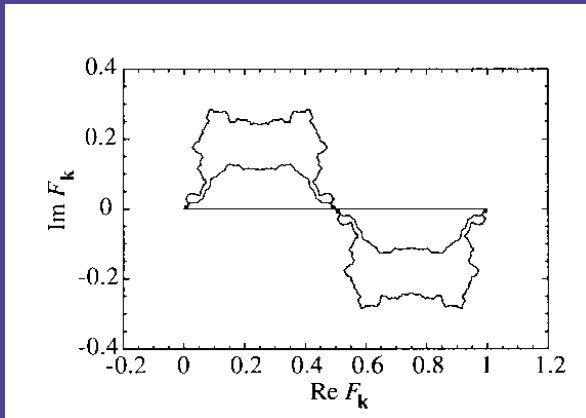
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The hydrodynamic modes have cumulative functions

$$F_{\mathbf{k}}(\theta) \equiv \lim_{t \rightarrow \infty} \frac{\int_0^\theta d\theta' \exp\{i\mathbf{k} \cdot [\mathbf{r}_t(\theta') - \mathbf{r}_0(\theta')]\}}{\int_0^{2\pi} d\theta' \exp\{i\mathbf{k} \cdot [\mathbf{r}_t(\theta') - \mathbf{r}_0(\theta')]\}}$$





(LHF) $k_x = 0.0, 0.5, 0.9$ ($k_y = 0$). The interdisk distance is $d = 2.3$ (the disk radius is unity). (RHF) Filled circles.





Entropy Production

For the Multi-Baker Map, given collections of cylinder sets of widths $1/3^l$ and $1/3^{l+1}$, the time-dependent entropy production rate in the n th unit square is given by

$$\Delta_i S_\tau(n) = \sum_{\omega_1, \dots, \omega_{l+1}} \Delta G_{\tau+1}[n, y(\omega_1, \dots, \omega_{l+1})] \\ \times \log \frac{3 \Delta G_{\tau+1}[n, y(\omega_1, \dots, \omega_{l+1})]}{\Delta G_{\tau+1}[n, y(\omega_1, \dots, \omega_l)]}$$





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Perform the gradient expansion

$$F_k(y) = y + ikT(y) + \mathcal{O}(k^2)$$



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$$\begin{aligned}\Delta_i S_\tau(n) &\approx \frac{\chi_k^{2\tau}}{2} \{2k \operatorname{Im}[a_k \exp(ikn)] + \mathcal{O}(k^2)\}^2 \\ &\quad \times [3^{l+1} \sum \Delta T(\omega_1, \dots, \omega_{l+1})^2 - \\ &\quad 3^l \sum \Delta T(\omega_1, \dots, \omega_l)^2] \\ &= \frac{\chi_k^{2\tau}}{3} \{2k \operatorname{Im}[a_k \exp(ikn)] + \mathcal{O}(k^2)\}^2\end{aligned}$$





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This expression agrees with the phenomenological rate of entropy production for a one-dimensional diffusive system

$$d_i S_t(r) = \frac{\mathcal{D}}{c_t(r)} \left[\frac{\partial c_t(r)}{\partial r} \right]^2$$



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Entropy Production of Diffusion and beyond

The formula derived for the multi-baker map is valid for entropy production in different classes of diffusive processes, including **tagged particle diffusion** for quasi-periodic systems.

The key concept is an appropriate definition of the *hydrodynamic measure* determined by the fractal properties of microscopic hydrodynamic modes.

The extension to other transport processes is under progress, starting with **viscosity** .



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