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THE FRACTALITY OF THE HYDRODYNAMIC MODES OF DIFFUSION

Pierre GASPARD
Center for Nonlinear Phenomena and Complex Systems,
Université Libre de Bruxelles, Code Postal 231,
Campus Plaine, B-1050 Brussels, Belgium
gaspard@ulb.ac.be

Transport by normal diffusion can be decomposed into hydrodynamic modes which relax exponentially toward the equilibrium state. In chaotic systems with two degrees of freedom, the fine scale structures of these modes are singular and fractal, characterized by a Hausdorff dimension given in terms of Ruelle's topological pressure. For long-wavelength modes, the Hausdorff dimension is related to the diffusion coefficient and the Lyapunov exponent. In the infinite-wavelength limit, the hydrodynamic modes lead to the nonequilibrium steady states, which also present a singular character. This singular character is a consequence of the mixing property of the dynamics. These results are illustrated with several systems such as the hard-disk and Yukawa-potential Lorentz gases.

I. INTRODUCTION

A fundamental problem of statistical mechanics is to derive the macroscopic equations of a fluid such as the Navier-Stokes equations, the heat equation or the diffusion equation from the underlying Newtonian dynamics of the particles composing the fluid. On the way from the microscopic dynamics to the macroscopic phenomena, a central role is played by the so-called hydrodynamic modes. These modes describe the collective motions of fluids with periodic inhomogeneities in space relaxing as exponential (or oscillatory exponential) functions in time toward the state of thermodynamic equilibrium. The importance of the hydrodynamic modes holds in the fact that they are associated with the locally conserved quantities: the energy, the momentum, and the masses or numbers of the conserved particles.

For the phenomenological diffusion equation

$$\partial_t \, n = \mathcal{D}\nabla^2 n \; , \tag{1}$$

where n is the concentration or density of tracer particles in the fluid and $\mathcal{D}$ is the diffusion coefficient, the hydrodynamic modes of diffusion are the special solutions

$$n(\mathbf{r},t) \sim e^{i\mathbf{k}\cdot\mathbf{r}} \, e^{s\,t} \; , \qquad \text{with} \quad s = -\mathcal{D}\mathbf{k}^2 \; , \tag{2}$$

where $\mathbf{k}$ is the wavenumber of the mode and the variable $s = \text{Re}\ s + i\text{Im}\ s$ gives the damping rate $-\text{Re}\ s$ and the frequency $\text{Im}\ s$ of the mode. We notice that the rate variable s is given by an eigenvalue problem for the operator in the right-hand side of the evolution equation, here Eq. (1). The relation between the rate variable s and the wavenumber $\mathbf{k}$ is the so-called dispersion relation, which characterizes the physical processes of wave propagation and relaxation. The knowledge of the dispersion relations provides the values of the transport coefficients such as the diffusion coefficient.

This is the way the transport coefficients are derived from kinetic equations such as the Boltzmann equation since the pioneering work by Hilbert [1], Chapman [2], and Enskog [3] (see Refs. [4–6]).

An example of such treatment is for the random Lorentz gas of independent particles in elastic collisions on hard disks of radius a. These scatterers are randomly located according to a Poisson distribution on the plane with the uniform density $n_{\rm d}$. In the dilute gas limit, $n_{\rm d}a^2 \ll 1$, the phase-space probability density $f(\mathbf{r},\varphi)$ that a tracer particle is located at the position $\mathbf{r}$ with the velocity $\mathbf{v} = v(\cos\varphi, \sin\varphi)$ evolves in time according to the Boltzmann-Lorentz equation [7]

$$\partial_t \, f + \mathbf{v}\cdot\boldsymbol{\nabla} f = \frac{n_{\rm d}av}{2}\int_{-\pi}^{+\pi} d\varphi' \left| \sin\frac{\varphi-\varphi'}{2}\right| \left[f(\mathbf{r},\varphi') - f(\mathbf{r},\varphi)\right] \; . \tag{3}$$

This kinetic equation admits special solutions of the form:

$$f(\mathbf{r},\varphi,t) \sim e^{i\mathbf{k}\cdot\mathbf{r}} \, e^{s\,t} \; , \tag{4}$$

with wavenumber $\mathbf{k}$. The dispersion relations of these modes are depicted in Fig. 1. At vanishing wavenumber, the rates are given by

$$\mathbf{k} = 0 \ : \qquad s = \frac{8j^2}{1-4j^2}\, n_{\rm d} a v \qquad (j = 0, 1, 2, ...) \ . \tag{5}$$

The branch such as $s = 0$ for $\mathbf{k} = 0$ corresponds to the diffusive mode for which $s = -\mathcal{D}\mathbf{k}^2 + O(\mathbf{k}^4)$ with the diffusion coefficient

$$\mathcal{D} = \frac{3v}{16 a n_{\rm d}} \ . \tag{6}$$

The other branches with larger damping rates correspond to the kinetic modes describing faster transients.

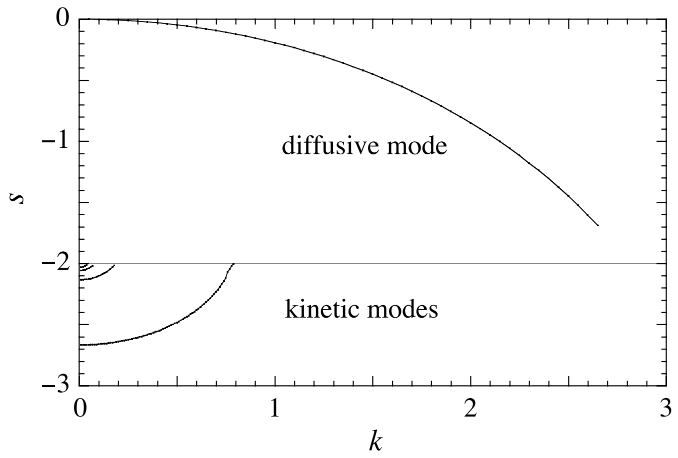

FIG. 1: Spectrum of the Boltzmann-Lorentz kinetic equation (3) for the random hard-disk Lorentz gas: rate variable s versus wavenumber $k = \|\mathbf{k}\|$. The disks are randomly distributed in the plane according to a Poisson distribution.

II. THE HYDRODYNAMIC MODES OF DIFFUSION IN PERIODIC LORENTZ GASES

The Boltzmann-Lorentz kinetic equation is only valid in the dilute-gas limit and for a statistical ensemble of configurations of the scatterers. A fundamental problem is to construct the hydrodynamic modes directly from the underlying microscopic dynamics in order to go beyond the restrictions on the use of typical kinetic equations.

Recently, it has been possible to carry out this construction for two-dimensional periodic Lorentz gases which conserve energy and preserve phase-space volumes according to Liouville's theorem. Two examples have been treated in detail:

(1) The hard-disk Lorentz gas on a triangular lattice, which has a finite and positive diffusion coefficient and is fully chaotic in the finite-horizon regime, as proved by Bunimovich and Sinai [8].

(2) The Yukawa-potential Lorentz gas on a square lattice, which is ruled by the Hamiltonian:

$$H = \frac{p_x^2 + p_y^2}{2m} - \sum_{\mathbf{l} \in Z^2} \frac{e^{-\alpha\|\mathbf{r}-\mathbf{l}\|}}{\|\mathbf{r}-\mathbf{l}\|} \ . \tag{7}$$

This system is fully chaotic and diffusive if the energy is larger than some value, as proved by Knauf [9].

The construction of the diffusive modes can be formulated by reducing the flow $\mathbf{X}_t = \mathbf{\Phi}^t(\mathbf{X}_0)$ with $\mathbf{X} = (\mathbf{r}, \varphi)$ to the Birkhoff-Poincaré map:

$$\begin{cases} \mathbf{x}_{n+1} = \boldsymbol{\phi}(\mathbf{x}_n) \ , \\ t_{n+1} = t_n + T(\mathbf{x}_n) \ , \\ \mathbf{l}_{n+1} = \mathbf{l}_n + \mathbf{a}(\mathbf{x}_n) \ , \end{cases} \tag{8}$$

where $\mathbf{x}_n$ are for instance the Birkhoff coordinates of the tracer particle at collision with a hard disk. $T(\mathbf{x})$ is the first-return time function and $\mathbf{l}_n \in \mathcal{L}$ is a vector of the lattice $\mathcal{L}$, pointing to the lattice cell where the particle is located. The function $\mathbf{a}(\mathbf{x})$ is the lattice vector of the jump of the tracer particle from cell to cell or from collision to collision.

Similarly, the Frobenius-Perron operator of the flow

$$f_t(\mathbf{X}) = f_0(\mathbf{\Phi}^{-t}\mathbf{X}) \;, \tag{9}$$

can be reduced to a Frobenius-Perron operator for the map (8). After a spatial Fourrier transform introducing the wavenumber $\mathbf{k}$ and a temporal Laplace transform introducing the rate variable s, the Frobenius-Perron operator of the map is given by

$$\left(\hat{R}_{\mathbf{k},s}u\right)(\mathbf{x}) = e^{-sT(\boldsymbol{\phi}^{-1}\mathbf{x})-i\mathbf{k}\cdot\mathbf{a}(\boldsymbol{\phi}^{-1}\mathbf{x})}u(\boldsymbol{\phi}^{-1}\mathbf{x}) \;. \tag{10}$$

Formally, the diffusive mode $\psi_{\mathbf{k}}(\mathbf{x})$ is an eigenstate of the operator (10) corresponding to the unit eigenvalue:

$$\hat{R}_{\mathbf{k},s_{\mathbf{k}}}\psi_{\mathbf{k}} = \psi_{\mathbf{k}} \;. \tag{11}$$

This eigenvalue condition constrains the rate variable s to become a function $s_{\mathbf{k}}$ of the wavenumber $\mathbf{k}$ [10]. This rate is a Pollicott-Ruelle resonance which gives the dispersion relation of diffusion:

$$s_{\mathbf{k}} = -\mathcal{D}\mathbf{k}^2 + O(\mathbf{k}^4) \;, \tag{12}$$

where the diffusion coefficient $\mathcal{D}$ is given by the Green-Kubo formula [11, 12]. Higher-order Burnett and super-Burnett coefficients can also be obtained [11–13]. The method based on the Frobenius-Perron operator yields the dispersion relation of diffusion in general.

A remarkable result is that the eigenstate $\Psi_{\mathbf{k}}(\mathbf{X})$ is not a function but a singular distribution with a cumulative function presenting fractal properties [14, 15]. The cumulative function of the diffusive mode $\Psi_{\mathbf{k}}$ can be constructed by first noticing that the dispersion relation of diffusion is equivalently given by the Van Hove formula as

$$s_{\mathbf{k}} = \lim_{t\to\infty}\frac{1}{t}\ln\langle e^{i\mathbf{k}\cdot(\mathbf{r}_t-\mathbf{r}_0)}\rangle \;, \tag{13}$$

where $\mathbf{r}_t$ is the position of the tracer particle issued from the initial position $\mathbf{r}_0$ and $\langle\cdot\rangle$ denotes the average over an ensemble of initial conditions. The choice of this ensemble is arbitrary as long as the mixing condition is satisfied. In this framework, the cumulative function is given by

$$F_{\mathbf{k}}(\theta) = \lim_{t\to\infty}\frac{\int_0^{\theta} e^{i\mathbf{k}\cdot(\mathbf{r}_t-\mathbf{r}_0)_{\theta'}}\,d\theta'}{\int_0^{2\pi} e^{i\mathbf{k}\cdot(\mathbf{r}_t-\mathbf{r}_0)_{\theta'}}\,d\theta'} \;, \tag{14}$$

where the integral is performed over an initial position and velocity having an angle θ with the horizon axis around the center of a scatterer. The cumulative function forms a curve in the complex plane $(\mathrm{Re}\,F_{\mathbf{k}}, \mathrm{Im}\,F_{\mathbf{k}})$. This curve has some fractal structure as seen in Fig. 2.

In Ref. [14], it was shown that, in fully chaotic systems, the Hausdorff dimension D_{H} of these curves in the complex plane is given by the root of the equation:

$$P(D_{\mathrm{H}}) = D_{\mathrm{H}}\;\mathrm{Re}\,s_{\mathbf{k}} \;, \tag{15}$$

where $s_{\mathbf{k}}$ is the dispersion relation of diffusion (12), while

$$P(\beta) \equiv \lim_{t\to\infty}\frac{1}{t}\ln\langle|\Lambda_t|^{1-\beta}\rangle \;, \tag{16}$$

is the Ruelle topological pressure function, i.e., the generating function of the stretching factors $|\Lambda_t| > 1$ associated with each trajectory of the system. We notice that the positive Lyapunov exponent is given by

$$\lambda^+ = -\frac{dP}{d\beta}(1) \;, \tag{17}$$

while $P(1) = 0$. Equation (15) generalizes a formula obtained by Bowen for the Hausdorff dimension of fractal invariant sets such as the Julia sets of complex analytic maps [16].

Using Eqs. (15), (12), and (17), the Hausdorff dimension is given at low wavenumbers by

$$D_{\mathrm{H}}(\mathbf{k}) = 1 + \frac{\mathcal{D}}{\lambda^+}\,\mathbf{k}^2 + O(\mathbf{k}^4) \;, \tag{18}$$

in terms of the diffusion coefficient $\mathcal{D}$ and the positive Lyapunov exponent λ^+. Reciprocally, the diffusion coefficient can be obtained from the Hausdorff dimension and the positive Lyapunov exponent as

$$\mathcal{D} = \lambda^+\;\lim_{\mathbf{k}\to 0}\frac{D_{\mathrm{H}}(\mathbf{k})-1}{\mathbf{k}^2} \;. \tag{19}$$

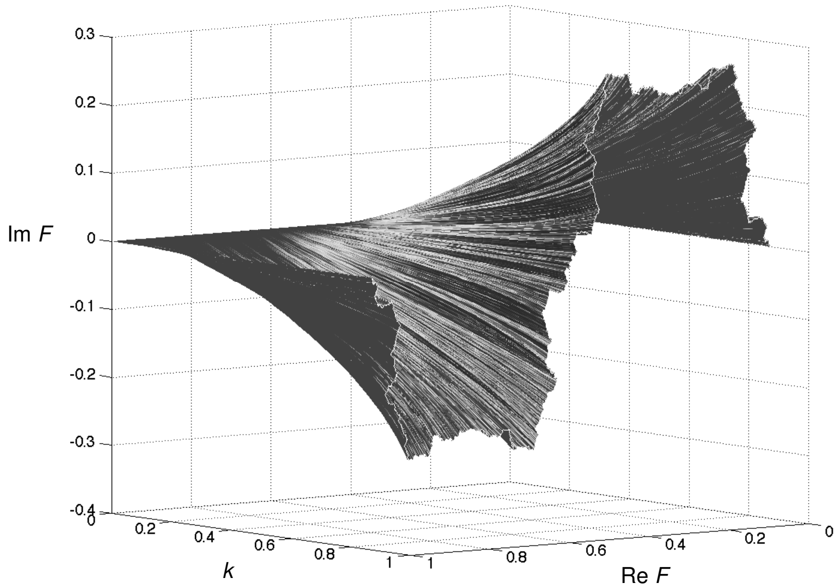

FIG. 2: Cumulative function (14) of the hydrodynamic modes of diffusion in the periodic hard-disk Lorentz gas versus the wavenumber $\mathbf{k} = (k, 0)$ of magnitude varying in the interval $0 \leq k < 0.9$. The disks form a triangular lattice, their centers are separated by the distance $d = 2.3$, and their radius is unity.

III. THE NONEQUILIBRIUM STEADY STATES OF DIFFUSION IN PERIODIC LORENTZ GASES

The nonequilibrium steady states corresponding to a gradient $\mathbf{g}$ of particle density between two reservoirs or chemiostats separated by an arbitrarily large distance can be derived from the diffusive modes $\Psi_{\mathbf{k}}$ according to

$$\Psi_{\mathbf{g}} \;=\; -\mathrm{i}\, \mathbf{g} \cdot \frac{\partial \Psi_{\mathbf{k}}}{\partial \mathbf{k}}\Big|_{\mathbf{k}=0} \, . \tag{20}$$

It has been shown [12] that, for Lorentz gases, this nonequilibrium steady state is given by

$$\Psi_{\mathbf{g}}(\mathbf{X}) \;=\; \mathbf{g} \cdot \left[\mathbf{r}(\mathbf{X}) + \int_0^{-\infty} \mathbf{v}(\mathbf{\Phi}^t \mathbf{X}) \; dt \right] \, . \tag{21}$$

Here again, this density is not a function but defines a singular distribution which can be represented by its cumulative function

$$T_{\mathbf{g}}(\theta) = \int_0^{\theta} d\theta' \; \Psi_{\mathbf{g}}(\mathbf{X}_{\theta'}) \, , \tag{22}$$

as depicted in Fig. 3. It has been shown in Ref. [11] that the average current of particles in the nonequilibrium steady state (21) obeys Fick's law. The reason is that the Green-Kubo formula is recovered after averaging the microscopic current given by the particle velocity $\mathbf{v}(\mathbf{X})$ over the steady state (21). Indeed, the second term in Eq. (21) is a part of the Green-Kubo formula while the first term has a vanishing contribution [11, 12].

An important remark is that the density of a nonequilibrium steady state of diffusion remains a function as far as the two reservoirs, between which the gradient of tracer particles is established, are at finite distance from each other. This density is highly complicated and transforms itself from a function to a singular distribution in the limit of an arbitrarily large separation between the reservoirs while keeping the gradient constant.

Finally, using the previous results and, especially, the singular steady state (21), it has been shown in Ref. [17] that, starting from a coarse-grained entropy, the leading term of the entropy production behaves as expected by the irreversible thermodynamics of diffusive processes. This result is an *ab initio* derivation of the entropy production from the underlying microscopic dynamics, which has been possible to carry out thanks to the explicit construction of the hydrodynamic modes (14) and the nonequilibrium steady state (21) in consistency with the Green-Kubo formula and Fick's law.

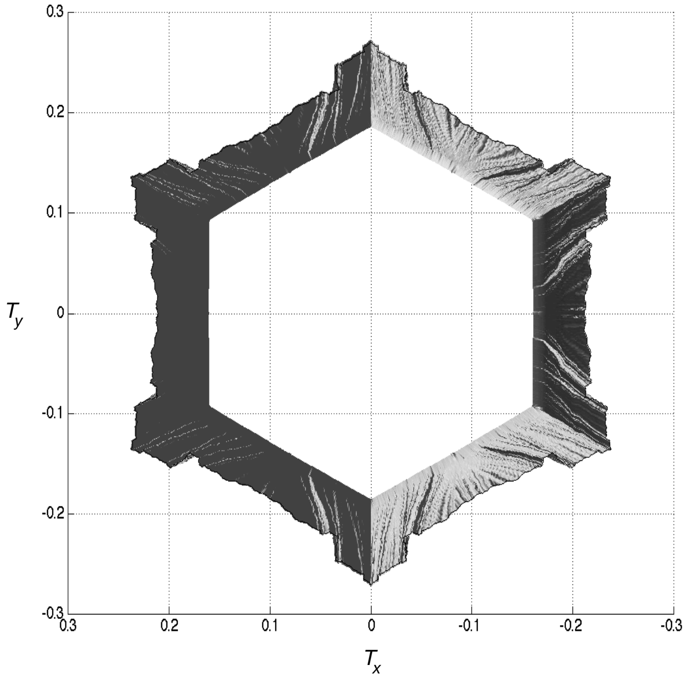

FIG. 3: Cumulative functions (22) of the nonequilibrium steady states of diffusion in the periodic hard-disk Lorentz gas in the plane of the quantities $T_x(\theta)$ and $T_y(\theta) - T_y(\pi/2)$ (where θ is the angle of the initial position on a disk). The third dimension of the plot is the interdisk gap w. The scatterers are disks of unit radius forming a triangular lattice of finite horizon $0 \leq w < (4/\sqrt{3}) - 2$.

IV. CONCLUSIONS

In this paper, we have shown how the hydrodynamic modes of diffusion as well as the associated nonequilibrium steady states can be explicitly constructed from the underlying microscopic dynamics in periodic Lorentz gases. This construction extends previous work on multibaker maps [12, 18–20]. The construction is based on a formulation in terms of the Frobenius-Perron operator, their eigenstates, and their corresponding Pollicott-Ruelle resonances. In the periodic Lorentz gases, the leading Pollicott-Ruelle resonance gives the dispersion relation of diffusion in consistency with the Green-Kubo and Van Hove formulae. The cumulative functions of the hydrodynamic modes form fractal curves in the complex plane. The Hausdorff dimension of these curves is given in terms of the Ruelle topological pressure, establishing the chaos-transport relationship (19) in the present context.

The derivation of the basic phenomenology of the irreversible processes of diffusion turns out to be possible for the deterministic dynamics of the periodic Lorentz gases at the price that the phase-space densities of the hydrodynamic modes (11) and of the nonequilibrium steady states (21) are given by singular distributions instead of functions.

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