Kolya and me: A scientific collaboration

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In memory of Kolya: a friend and teacher

Abstract

I will give an overview of some of my work with Kolya, beginning in 1992 and left incomplete by his tragic untimely death.

This falls into three groups:

1. Electrical Conduction in a thermostated Sinai billiard.

2. Shear flow in a fluid driven by Maxwell-demon boundaries.

3. Thermalization of the notorious piston.

Introduction

Equilibrium statistical mechanics is a mathematically beautiful and physically successful theory. It uses Gibbs measures on the phase space of (classical) macroscopic systems to describe and predict properties such as specific heat, phase transitions, etc., in equilibrium. These measures, $\mu(dX)$, $X = (q_1, \ldots, v_1, \ldots, v_N), q_i \in \Lambda \subset \mathbb{R}^d, v_i \in \mathbb{R}^d$ are stationary under the time evolution given by the dynamics generated by their Hamiltonian, $H(X)$: they have a uniform density on the energy surfaces, $H(X) =$ Const. , e.g. the microcanonical or canonical ensembles.

The reason this procedure works so well for equilibrium systems is roughly speaking due to the fact that “ almost all” phase points on the energy surface correspond to equilibrium states. Strict mathematical ergodicity is nice but not essential for this.

A goal of nonequilibrium statistical mechanics is to find measures which will describe the nonequilibrium stationary states (NESS) of systems in which there are flows, such as an electric current. To do that one needs to consider either: i) open systems, i.e. ones in contact with infinite reservoirs, usually modeled by adding stochastic terms to the Hamiltonian evolution, or ii) closed systems with non-Hamiltonian dynamics, usually modeled by adding deterministic non-Hamiltonian terms to the Hamiltonian dynamics. When done judiciously, the resulting stationary measures will be candidates to model NESS of physical interest.

My work with Kolya involved two situations of type (ii) as well as one time dependent case.

Gaussian thermostated systems

A much studied example of such non-Hamiltonian dynamics is one with a Gaussian thermostat which keeps the kinetic energy of the system constant. While this dynamics is not very physical, it is mathematically interesting and can be related in many cases to physical behavior. In particular, it has led to rigorous theorems, such as the Gallavotti-Cohen fluctuation theorem for Anosov flows which appear to apply also to physical systems with chaotic Hamiltonian dynamics. Such a system of particles (electrons) moving among a fixed array of periodic scatterers under the action of an external field was the subject of my first paper with Kolya.

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Steady-State Electrical Conduction in the Periodic Lorentz Gas

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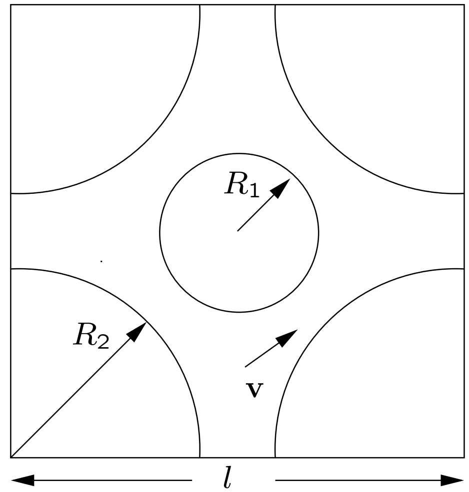
Dedicated to Elliott Lieb

Abstract. We study nonequilibrium steady states in the Lorentz gas of periodic scatterers when an electric external field is applied and the particle kinetic energy is held fixed by a "thermostat" constructed according to Gauss' principle of least constraint (a model problem previously studied numerically by Moran and Hoover). The resulting dynamics is reversible and deterministic, but does not preserve Liouville measure. For a sufficiently small field, we prove the following results: (1) existence of a unique stationary, ergodic measure obtained by forward evolution of initial absolutely continuous distributions, for which the Pesin entropy formula and Young's expression for the fractal dimension are valid; (2) exact identity of the steady-state thermodynamic entropy production, the asymptotic decay of the Gibbs entropy for the time-evolved distribution, and minus the sum of the Lyapunov exponents; (3) an explicit expression for the full nonlinear current response (Kawasaki formula); and (4) validity of linear response theory and Ohm's transport law, including the Einstein relation between conductivity and diffusion matrices. Results (2) and (4) yield also a direct relation between Lyapunov exponents and zero-field transport (= diffusion) coefficients. Although we restrict ourselves here to dimension $d = 2$, the results carry over to higher dimensions and to some other physical situations: e.g. with additional external magnetic fields. The proofs use a well-developed theory of small perturbations of hyperbolic dynamical systems and the method of Markov sieves, an approximation of Markov partitions.

I. Physical Discussion and Statement of Results

(a) *Introduction.* We consider in this paper a dynamical system which corresponds to the motion of a single particle between a finite number of fixed, disjoint, convex scatterers in a periodic domain of the plane $\mathbb{R}^2$. As in the previous works [2, 3], the particle changes its velocity at moments of collision according to the usual law of elastic reflection, but, unlike there, the particle motion between collisions is not the free one at constant velocity. Instead, the motion between collisions is governed by



Moran-Hoover model

The equations describing the motion of the particle, including elastic scattering with the obstacles, are:

$$\begin{cases} \dot{\mathbf{q}} &= \mathbf{v} \\ \dot{\mathbf{v}} &= \mathbf{E} - \alpha(\mathbf{v})\mathbf{v} + F_{obs}(\mathbf{q}) \\ \alpha &= \frac{(\mathbf{v}\cdot\mathbf{E})}{(\mathbf{v}\cdot\mathbf{v})} \end{cases} \tag{1}$$

where $(\cdot)$ represents the usual scalar product in $\mathbb{R}^2$, and we have set the mass of the particle equal to unity. It follows that

$$\frac{1}{2}\frac{d}{dt}\ v^2 = \mathbf{E}\cdot\mathbf{v} - \alpha v^2 = 0. \tag{2}$$

This dynamics does not conserve phase space volume: div $\dot{\mathbf{v}} = -\alpha$.

A snapshot of the density of trajectories crossing the Poincaré plane for a very similar model studied by Hoover and Posch. The density would be uniform for $\mathbf{E} = 0$, corresponding to the microcanonical ensemble.

Inspired by these pictures of singular measures, Chernov, Eyink, L., Sinai proved for small values of $\mathbf{E}$ (and magnetic field $\mathbf{B}$), that this system has a unique stationary SRB measure which is approached as $t \to \infty$ from any initial measure which is absolutely continuous w.r.t. Lebesgue measure.

This SRB measure, $\mu_{\mathbf{E}}^{+}$, is singular w.r.t. Lebesgue measure. Its Hausdorff dimension is given for small $E = |\mathbf{E}|$ by

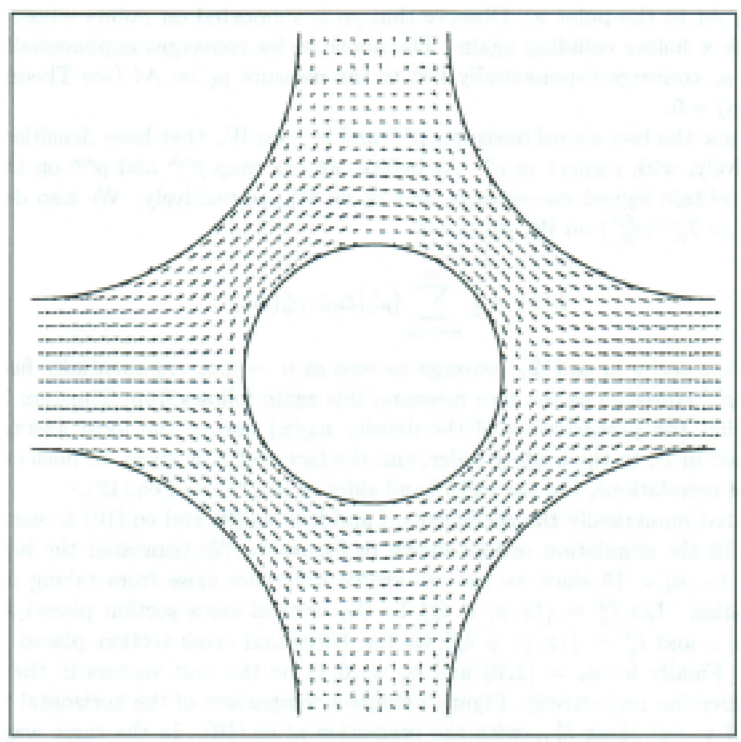
$$HD\left(\mu_{\mathbf{E}}^{+}\right) = 3 - \frac{\bar{\mathbf{J}} \cdot \mathbf{E}}{h_0} + o(E^2), \tag{3}$$

where h_0 is the K-S entropy at zero field and the average current $\mathbf{J}$ is given by

$$\mathbf{J} = \mu_{\mathbf{E}}^{+}(\mathbf{v}) = \underline{\boldsymbol{\sigma}}_0 \mathbf{E} + o(E). \tag{4}$$

Here, $\underline{\boldsymbol{\sigma}}_0$ is the conductivity tensor; it is equal to the diffusion tensor $\underline{\mathbf{D}}$ in zero field, computed by Bunimovich, Chernov and Sinai. This is in accord with the Einstein-Green-Kubo relation.

It was also shown later by Bonetto, Chernov, Korepanov, L. (BCKL) that despite the singular nature of $\mu^{+}_{\mathbf{E}}$, its projections on space coordinates are absolutely continuous. This is in agreement with results found by Bonetto, Kupiainen, L. about projections of SRB measures. Here is a picture of the flow with the field in the x-direction, $E = 0.1$, in appropriate units ($m = |\mathbf{v}| = L = 1$).



The proof by CELS makes strong use of the fact that in the absense of an external field $\mathbf{E}$, when the dynamics is Hamiltonian, this system is uniformly hyperbolic. This means unfortunately that there are no exact results for this system when the number of electrons, N, moving in the billiard is greater than 1, when the system is not uniformly hyperbolic in the absence of an external field.

Numerical and heuristic results strongly suggest however that this system has a unique NESS for $|\mathbf{E}| \in [0, E_0]$ for all N. This was first noted in Bonetto, Deems, L., Ricci (BDLR).

BDLR also introduced an approximate description in which the obstacles are replaced by random scatterings, as described below.

We (Bonetto, Chernov, Korepanov, L.) returned to the study of this system in 2010. Surprisingly we found in very high precision numerical simulations that when $|\mathbf{E}|$ is small, say $|\mathbf{E}| \leq .2$, the deterministic mechanical system has a NESS speed distribution which is independent of the shape of the billiard table. In fact, we argue that this speed distribution coincides, in the limit $\mathbf{E} \to 0$, with that obtained from the NESS of the BDLR stochastic model which can be computed explicitly, see Figures.

Multiparticle system moving among fixed scatterers subject to an external field, $\mathbf{E}$, and a Gaussian thermostat.

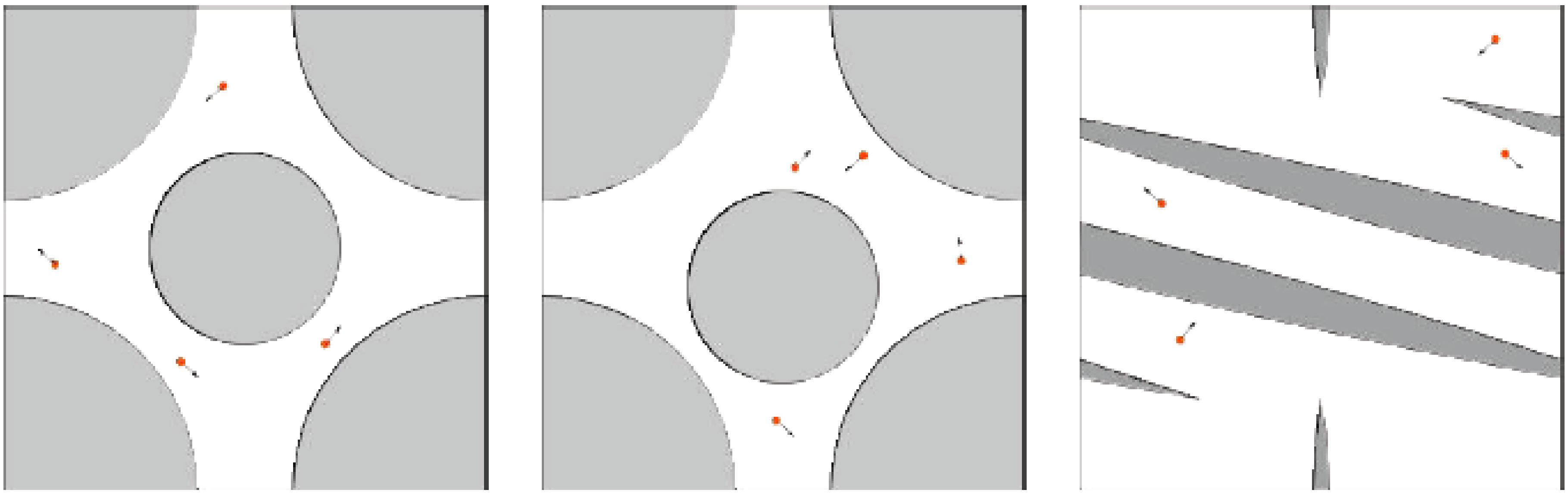


Table A Table B Table C

Different Sinai billiard tables.

The equations of motion of the system, consisting of N particles of mass 1 in a unit 2D torus, are

$$\begin{cases} \dot{\mathbf{q}}_i = \mathbf{v}_i \\ \dot{\mathbf{v}}_i = \mathbf{E} - \alpha(\mathbf{V}, K)\mathbf{v}_i + \mathbf{F}_i \end{cases} \qquad i = 1, 2, \ldots N \tag{5}$$

where $\mathbf{E}$ is the external field,

$$\alpha(\mathbf{V}, K) = \frac{(\mathbf{E} \cdot \mathbf{J})}{K}, \qquad \mathbf{J} = \sum_i \mathbf{v}_i, \qquad K = \sum_i |\mathbf{v}_i|^2 \tag{6}$$

and $\mathbf{F}_i$ is an impulsive change in the momentum of the i-th particle caused by its collision with a fixed scatterer, as in the figure. The term $\alpha(\mathbf{V}, K)$ represents the Gaussian thermostat which keeps K fixed. We may therefore set $K = N$. I shall refer to this system as the mechanical one (designated by M).

In the stochastic model (designated by S) the equations of motion are the same as (5) **except** that $\mathbf{F}_i$ now represents "random" scatterings by "virtual" collisions which conserve energy but not momentum. More precisely we imagine that each particle will suffer a collision in which the direction of its velocity changes according the rule

$$\mathbf{v}' = \mathbf{v} - 2\hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \mathbf{v}) \tag{7}$$

where $\hat{\mathbf{n}}$ is a unit vector in the direction of the momentum transfer from $\mathbf{v}$ to $\mathbf{v}'$. The direction of $\hat{\mathbf{n}}$ is random subject to the constraint $(\hat{\mathbf{n}} \cdot \mathbf{v}) < 0$. (This corresponds to the "Boltzmann-Grad limit" of scatterers with density ρ and diameter a with $\rho \to \infty$, $a \to 0$, $\rho a = l^{-1}$, the inverse of the mean-free path, staying finite.)

It is to be noted that for either M or S, the Gaussian thermostat induces a “long range,” “mean field” type of interaction between the particles: the speed gained by any particle due to the electric field has to be compensated by loss of speed in *all* the other particles due to the thermostated “friction” α.

Using S, the "master" equation describing the time evolution of the N-particle velocity distribution function, which is independent of the positions $\mathbf{q}_i$ is, given by

$$\begin{aligned}\frac{\partial W(\mathbf{V},t)}{\partial t} &= -\sum_{i=1}^{N}\frac{\partial}{\partial \mathbf{v}_i}\Big[\Big(\mathbf{E}-(\mathbf{E}\cdot\mathbf{j})\mathbf{v}_i\Big)W\Big] \\ &\quad+\sum_{i=1}^{N}\frac{1}{2}\int(\mathbf{v}_i'\cdot\hat{\mathbf{n}})\Big[W(\mathbf{V}_i',t;\mathbf{E})-W(\mathbf{V},t;\mathbf{E})\Big]\,d\hat{\mathbf{n}} \\ &= E\,\mathcal{B}(W)+\mathcal{C}(W) \qquad (8)\end{aligned}$$

where $\mathbf{j}=\mathbf{J}/K$

$$\mathbf{V}=(\mathbf{v}_1,\ldots,\mathbf{v}_i,\ldots,\mathbf{v}_N) \quad \text{and} \quad \mathbf{V}_i'=(\mathbf{v}_1,\ldots,\mathbf{v}_i',\ldots,\mathbf{v}_N), \qquad (9)$$

and $\mathbf{v}_i'$ is given in terms of $\mathbf{v}_i$ by (7).

In the rhs of (8), E is the magnitude of $\mathbf{E}$, i.e., $\mathbf{E} = E\mathbf{e}$ for a unit vector $\mathbf{e}$, and $\mathcal{C} = \sum_{i=1}^{N} \mathcal{C}_i$ is the sum of collision terms for the different particles. These occur independently and do not depend on E.

The master (Liouville) equation for the deterministic model would involve also the position coordinates $\mathbf{Q} = (\mathbf{q}_1, \ldots, \mathbf{q}_N)$ and have the form

$$\frac{\partial \tilde{W}(\mathbf{Q}, \mathbf{V}, t)}{\partial t} + \sum_{i=1}^{N} \mathbf{v}_i \frac{\partial \tilde{W}}{\partial \mathbf{q}_i} + \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{v}_i} \Big[\Big(\mathbf{E} - (\mathbf{E} \cdot \mathbf{j}) \mathbf{v}_i \Big) \tilde{W} \Big] = \delta_c W \qquad (10)$$

with $\delta_c W$ representing the collisions with the fixed convex obstacles.

We are interested in the properties of these systems for small E. In fact, we would like to consider the stationary state in the limit $E \to 0$.

NB: The NESS of the mechanical or of the stochastic model in the limit $\mathbf{E} \to 0$ is not the same as the stationary state for $\mathbf{E} = 0$. In fact for $\mathbf{E} = 0$ there is no interaction between the particles and the speed of each particle remains unchanged in time; it can be prescribed initially in an arbitrary fashion but the collisions (deterministic or stochastic) will randomize its direction.

When E is small the appropriate time scale for the change in the speed of the particles will be of order E^{-2}. On that time scale each particle will have undergone many collisions and so one may then expect to have an autonomous equation for the distribution of the speed. In order to see this we rescale the time, setting $t = \frac{\tau}{E^2}$. Writing $\widetilde{W}(\mathbf{V}, \tau; E) = W(\mathbf{V}, tE^2; E)$ we observe that it satisfies the rescaled equation

$$\frac{\partial \widetilde{W}(\mathbf{V}, \tau)}{\partial \tau} + E^{-1}\mathcal{B}\widetilde{W}(\mathbf{V}, t) = E^{-2}\mathcal{C}\widetilde{W}(\mathbf{V}, t) \tag{11}$$

We now assume that

$$\widetilde{W}(\mathbf{V}, \tau; E) = W^{(0)}(\mathbf{V}, \tau) + EW^{(1)}(\mathbf{V}, \tau) + E^2W^{(2)}(\mathbf{V}, \tau) + O(E^3)$$

This is a very strong assumption, in fact stronger than what we need but it makes the analysis much simpler. We believe that the final result can be justified with a more detailed analysis (cut short by Kolya's untimely death).

Replacing the above expansion in the equation we get that, for eq.(11) to make sense, we need

$$\begin{aligned}
\mathcal{C}\widetilde{W}^{(0)}(\mathbf{V},\tau) &= 0 && (12)\\
\mathcal{C}\widetilde{W}^{(1)}(\mathbf{V},\tau) &= \mathcal{B}\widetilde{W}^{(0)}(\mathbf{V},\tau) && (13)\\
\frac{\partial \widetilde{W}^{(0)}(\mathbf{V},\tau)}{\partial \tau} + \mathcal{B}\widetilde{W}^{(1)}(\mathbf{V},\tau) &= \mathcal{C}\widetilde{W}^{(2)}(\mathbf{V},\tau) && (14)
\end{aligned}$$

Surprisingly, one can actually find, after much sweat, the stationary solution of these equations, corresponding to the limit $\tau \to \infty$.

Setting $\mathbf{v}_i = (r_i, \theta_i)$ where $r_i = |\mathbf{v}_i|$ and the angle θ_i is taken with respect to the field direction which we can assume is in the x-direction, $\mathbf{V} = (\mathbf{R}, \boldsymbol{\Theta})$ we then find the stationary solution,

$$W(\mathbf{R}, \mathbf{\Theta}; E, N) = F_0(\mathbf{R}) + EF_1(\mathbf{R}, \mathbf{\Theta}) + o(E), \tag{15}$$

where

$$\bar{F}_0(\mathbf{R}) = \frac{1}{Z}\,\delta(K - N)\left[\sum_{i=1}^{N} r_i^3\right]^{-\frac{2N-1}{3}} \tag{16}$$

where Z is just the normalization

$$Z = \int_{\sum r_i^2 = N}\left[\sum_{i=1}^{N} r_i^3\right]^{-\frac{2N-1}{3}} \prod_{i=1}^{N} r_i\, dr_i, \tag{17}$$

and

$$F_1(\mathbf{R}, \mathbf{\Theta}; N) = (2N-1)\left[\sum_{i=1}^{N} r_i^3\right]^{-\frac{2N+2}{3}} \sum_{i=1}^{N} r_i c(\theta_i) \tag{18}$$

where $c(\theta_i)$ is computed explicitly.

To get the one particle marginal speed distribution $f_0(r; N)$ one has to integrate (16) over the variables $r_2, \ldots, r_N$. This has been done by Bonetto and Loss and gives, in the limit $N \to \infty$, the strikingly simple universal expression

$$\lim_{\mathbf{E}\to 0} \tilde{f}_{\mathbf{E}}(v) = \tilde{f}_0(v) = Cve^{-cv^3}, \quad v = |\mathbf{v}| \tag{19}$$

where

$$C = \frac{\sqrt{3}}{3}\frac{1}{\Gamma\left(\frac{2}{3}\right)^3} \approx 0.233, \tag{20}$$

$$c = \frac{2}{27}\frac{\sqrt{2}\pi^{\frac{3}{2}}3^{\frac{3}{4}}}{\Gamma\left(\frac{2}{3}\right)^3} \approx 0.536 \tag{21}$$

are determined uniquely by the requirements that

$$\int_0^\infty v^2 \tilde{f}_0(v)\, dv = \int_0^\infty \tilde{f}_0(v)\, dv = \frac{1}{2\pi}. \tag{22}$$

Self-consistent BE

The distribution (19) was actually first derived in BDLR by writing an autonomous non-linear self-consistent kinetic Boltzmann equation (BE) for $f(v,t)$. This is based on the intuitive idea that, $\mathbf{j} = \sum_{i=1}^{N} \mathbf{v}_i/N$, in eq.(5) will approach, in the limit $N \to \infty$, a deterministic value $\langle \mathbf{v} \rangle$. This yields then an equation for the one particle marginal with F_i stochastic

$$\frac{\partial}{\partial t} f(\mathbf{v},t) + \frac{\partial}{\partial \mathbf{v}} \left[\left(\mathbf{E} - \frac{\mathbf{E} \cdot \langle \mathbf{v} \rangle}{\langle |\mathbf{v}|^2 \rangle} \mathbf{v} \right) f(\mathbf{v},t) \right] = \frac{1}{l} \int_{\mathbf{v}\cdot\mathbf{n}<0} \frac{\mathbf{v}' \cdot \mathbf{n}}{2} \Big(f(\mathbf{v}',t) - f(\mathbf{v},t) \Big)\, d\mathbf{n} \tag{23}$$

Eq.(23) yields immediately that

$$\frac{d}{dt} \int |\mathbf{v}|^2 f(\mathbf{v},t)\, d\mathbf{v} = \frac{d}{dt} \, \langle |\mathbf{v}|^2 \rangle = 0 \tag{24}$$

so that if we chose $f(\mathbf{v},0)$ such that $\langle |\mathbf{v}(0)|^2 \rangle = 1$ we will have $\langle |\mathbf{v}(t)|^2 \rangle = 1$ for all t. The current $\langle \mathbf{v}(t) \rangle = \mathbf{j}$ will then have to be determined self-consistently from the solution of (23). This yields again (19) in the limit $E \to 0$.

We find numerically that (19) holds with high precision for both the mechanical and stochastic systems. We believe that it is indeed the exact stationary solution of the speed distribution of this system when $N \to \infty, E \to 0$.

The distribution (19) can also be related to the time rescaled $(v/t^{1/3})$ distribution of a single particle in a field E without thermostat, studied by Chernov and Dolgopyat.

Large field

When the field is large, the mechanical system behaves very differently from the stochastic one, with particle trajectories essentially "hugging" the obstacles. The stochastic one is of course always spatially uniform.

On the other hand we also find (numerically) that for $N >> 1$ the one-particle marginal velocity distribution of the stochastic model is very close to that obtained from the solution of a self-consistent Boltzmann equation (23) introduced in BDLR. This can actually be proven in the limit $N \to \infty$ (Bonetto, Carlen, Esposito, L, Marra).