
A new model for the transport of particles in a thermostatted system

Giancarlo Benettin* and Lamberto Rondoni†

Abstract

We introduce an elementary microscopic model for the free expansion of a gas from a smaller to a larger reservoir; a “pump” takes the particles back to the original reservoir, so as to maintain a stationary situation. The system is dissipative and thermostatted (with an elementary non Gaussian reversible thermostat). We consider here only the case of noninteracting particles. We identify a parameter in the system, playing the role of the field, and investigate numerically the usual transport properties, among them the proportionality of the current to the field for small fields, and the proportionality of the volume contraction rate to the product of field and current, in the same conditions. In spite of the simplicity of the model (and of the difficulty in the thermodynamical interpretation, the model being non interacting) we find apparently normal transport laws. We also make a particularly accurate test of the Gallavotti–Cohen fluctuation formula, which turns out to be always well satisfied (though fluctuations, in some conditions, are rather far from Gaussian). A leading idea of the paper is to look for the minimal requirements that a particle system should satisfy in order to give rise, at least formally, to normal transport.

Keywords: nonequilibrium, chaotic hypothesis, deterministic thermostat, fluctuations.

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1 Introduction

In the past few years, a considerable amount of work has been devoted to investigate the ergodic problem for systems in stationary non-equilibrium states (see, e.g. [PG98,GG99]). The purpose is to understand transport phenomena on the basis of the microscopic dynamics and, in particular, to identify the features of the microscopic (deterministic and reversible) dynamics which determine the normal macroscopic behavior. Since nonequilibrium systems in a steady state are necessarily thermostatted, for the thermostat too a microscopic model must be provided, and this is one of the most critical points of the question.

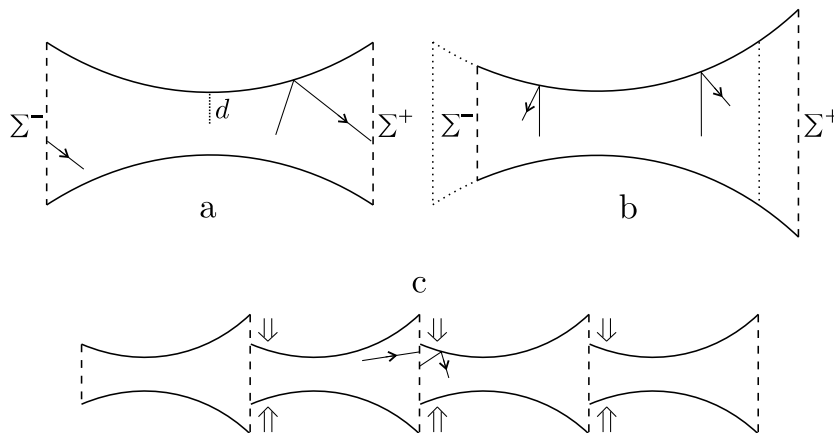
The transport phenomena which have been taken into consideration till now include the transport of charged particles in an electric field, the transport of heat in a temperature gradient, and the transfer of momentum in a viscous flow. A number of numerical studies have been published on several particle systems, like in Refs. [LLP98,BGG97,CL97,RM01], as well as on single particle ones, like in Refs. [LNRM,RKN00,BDL00,AACG99]. One particle systems (or equivalently, systems of several noninteracting particles) are of course less realistic than interacting particle systems. They are indeed good models for gases with mean free path larger than the characteristic length of the container, such as Knudsen gases, while their use in other physical situations is open to criticism. On the other hand, dealing with only a few degrees of freedom, one can afford much more accurate calculations than in the case of many particle systems, thus maximizing the significance of the calculations themselves. Moreover, it is always interesting, in our opinion, to know which are the minimal requirements on the microscopic dynamics, which lead nevertheless to regular macroscopic phenomena.

A theory for the nonequilibrium ergodic problem has been proposed a few years ago by Gallavotti and Cohen [GC95]. These authors have proposed the Anosov property of hyperbolic dynamical systems as the basis for the study of nonequilibrium statistical mechanical systems. The corresponding *physical* assumption, also known as “Chaotic Hypothesis” (CH), is that *a system in a stationary nonequilibrium state behaves, for what concerns transport properties, as a transitive Anosov system* (though in general it is not: similarly, equilibrium systems are almost never ergodic, but behave macroscopically as if they were). A consequence of the CH is the so-called “fluctuation formula”, which is an analytic expression involving the distribution of the fluctuations of the phase space contraction rate.

The purpose of this paper is twofold. On the one hand, we wish to introduce a model for an elementary transport phenomenon which (to our knowledge) has not been taken into consideration, namely the free expansion of a gas from a smaller to a larger reservoir. In our model, particles flow “geometrically”, as in billiards, from one reservoir to the other, and when they arrive, a “pump” takes them back to the original reservoir, so as to maintain a stationary situation. On the other hand, we wish to produce a model as elementary as possible, in particular for what concerns the thermostat, in the challenge to reach the maximal microscopic simplicity, which —formally, at least— yields a normal macroscopic behavior.

This paper is fully numeric, though theoretical results (essentially, hyperbolicity for the “closed model” treated below) could be produced, and will be the subject of future works [BLR]. Our results are the following:

- i. The current J is a linear function of the “field” ε for small ε , up to, in some conditions, a logarithmic correction (see below for the precise definition of ε). The phase space contraction rate is in turn proportional, for small ε , to the product εJ . This is guaranteed to be the case for Gaussian thermostats [CR98], while for our thermostat it is not and, indeed, for larger fields both laws get nonlinear.


 Figure 1: *The open model*

- ii. At low fields the support of the invariant measure (which is singular with respect to the Lebesgue measure) is the whole phase space, as for the SRB measure of transitive Anosov systems, while at higher fields it collapses onto a self-similar attractor.
- iii. Fluctuations obey, with great accuracy, the Gallavotti–Cohen fluctuation formula, though (in some cases) *large fluctuations are remarkably non Gaussian*. We are not aware of a similarly accurate critical check in other models, and interpret such a result as a significant confirmation of the Gallavotti–Cohen theory.
- iv. Hyperbolicity looks necessary: if we modify the model to remove hyperbolicity at zero field (the system remaining however ergodic, as flat billiards can be), the normal behavior at large time disappears. As in [LRB00], however, we observe an approximately normal transport for a long transient.

The simplicity of the model, which is fully geometric as billiards are and does not require solving differential equations, allows us to simulate quite long trajectories (occasionally more than 10^{11} billiard collisions) in a reasonable time. The corresponding large statistics in turn produces rather accurate results.

The paper is organized as follows: in Section 2 we define precisely our model. Section 3 reports the results for the current and the volume contraction, Section 4 is concerned with the support of the invariant measure, and Section 5 is devoted to the fluctuation formula. Finally, Section 6 contains a few further results and some concluding comments.

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2 The model

The model we propose, in its simplest version, is described in figure 1. For zero field it is a hyperbolic billiard, periodic in the horizontal direction, with elementary cell as in figure 1a. The upper and lower sides are arcs of circle of given radius r and amplitude $\varphi = 2 \arcsin r^{-1}$, at minimal distance $2d$ of each other. The billiard particle bounces elastically on them. If the particle exits the system from the left or right side of the cell, denoted respectively Σ^- and Σ^+ ,

it reappears in the obvious way on the opposite side. For nonzero field, figure 1b, the cell is made asymmetric by moving the ends of the arcs to the right (r and φ remaining unchanged), so as the ratio $\alpha = |\Sigma^+|/|\Sigma^-|$ between the sizes of Σ^+ and of Σ^- gets larger than one. The model is still periodic, see figure 1c, and periodicity is now realized by imposing the re-injection law

$$x' = x \mp l, \quad y' = \alpha^{\mp 1} y \quad (1)$$

on Σ^\pm , l denoting the length of the cell. This is a model for the free expansion of a gas from a smaller to a larger reservoir, followed by a compression (with external work), so as to maintain a stationary situation. The elementary microscopic mechanism which is expected to produce an average positive current is shown in figure 1b: the convex sides produce a forward and backward focusing of the particles, and for $\alpha > 1$ the forward focusing prevails.

Concerning the particle velocity $v = (v_x, v_y)$, we recall that the adiabatic compression of a gas produces a temperature increase. If we interpret the crossing of Σ^+ in our model as such a compression, we should associate a velocity increase to the crossing of Σ^+ . To keep the corresponding “temperature” fixed, a thermostat is necessary, and *the simplest microscopic implementation of the thermostat, is the elementary prescription that v^2 during the compression is kept constant*. This does not mean necessarily $v' = v$ (having denoted by v' the new velocity). Such a re-injection rule is in fact too simple, and as is easily checked, the combination of forward focusing and squeezing produces a collapse of the dynamics onto the forward central horizontal trajectory. To make such a trajectory unstable, one can change the ratio v_y/v_x by a factor $\beta > 1$ on Σ^+ , and β^{-1} on Σ^- , thus completing the re-injection law (1) by

$$v'_x = c v_x, \quad v'_y = c \beta^{\pm 1} v_y, \quad c^2 = \frac{v_x^2 + v_y^2}{v_x^2 + \beta^{\pm 2} v_y^2}. \quad (2)$$

The microscopic dynamics is easily seen to be reversible. The Jacobian \mathcal{J}^\pm of the map $\Psi^\pm : (x, y, v_x, v_y) \rightarrow (x', y', v'_x, v'_y)$ at Σ^\pm is easily computed, and the result is

$$\mathcal{J}^\pm = \frac{(\beta/\alpha)^{\pm 1}}{[1 + (\beta^{\pm 2} - 1) v_y^2]^{3/2}}; \quad (3)$$

so, to ensure dissipation i.e. Jacobian less than one for the crossing of Σ^+ (forward motion), it is sufficient to take $\beta < \alpha$. Our choice will be $\beta = \alpha^{1/2}$. Since v^2 is constant, we fix it to one. A convenient measure of the lack of symmetry in the model turns out to be

$$\varepsilon = \log \alpha,$$

which we identify with a “potential difference” between Σ^- and Σ^+ , or with a “field” acting on the system (field and potential difference cannot be distinguished in systems of fixed length). Let us remark that $\log \alpha$ coincides, up to a multiplicative constant, with the work done on a gas during an isothermal compression of a factor α .

The model described above will be called the “*open model*”, for it has open horizon. Many variants with closed horizon could be proposed. Among them, we chose the geometry represented in figure 2: the elementary cell is doubled, and in the middle a circular obstacle of radius $R > d$ is inserted. The two half-cells join continuously in the middle; as before, $\alpha > 1$ denotes the ratio between the sizes of the end sides Σ^\pm of the cell. For such a model, that we shall call the “*closed model*”, the re-injection rule of the velocity is less critical (see Section 5 for further comments). We used typically $\beta = \alpha^{1/2}$, for comparison with the open model, and occasionally other values of β , including $\beta = 1$ (i.e. $v' = v$).

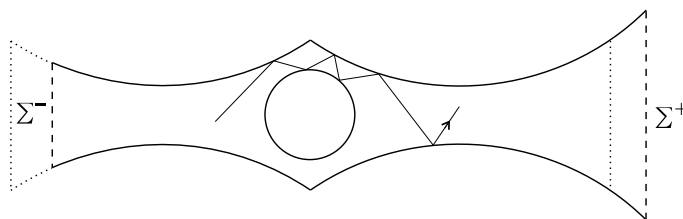


Figure 2: *The closed model.*

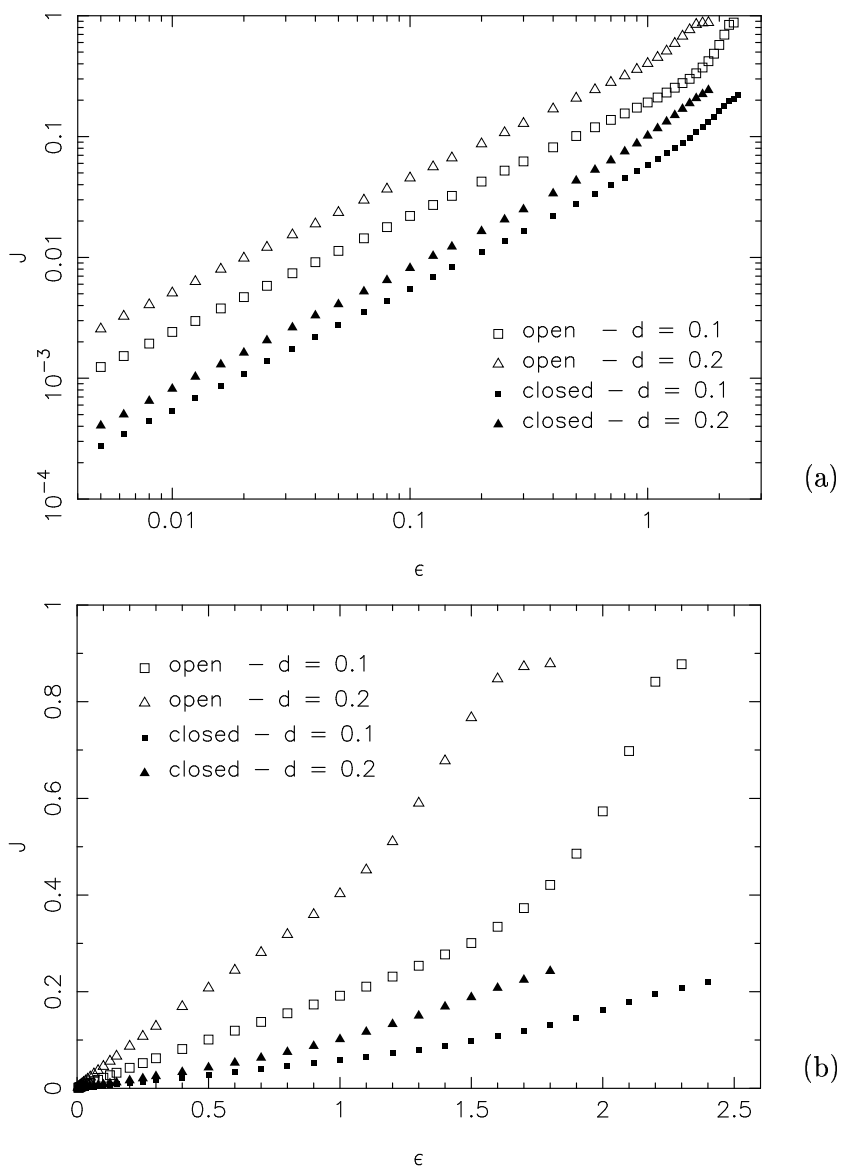


Figure 3: *The current J vs. the field ϵ , in linear (a) and logarithmic (b) scale.*

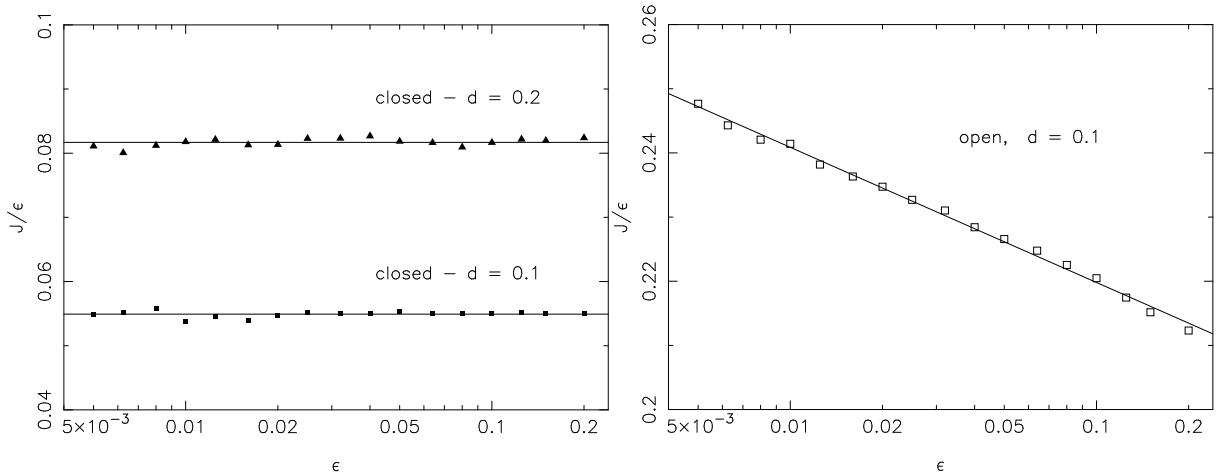


Figure 4: *The conductivity J/ε vs. ε , for the closed (left) and the open (right) models. Expanded vertical scale (same scale in the two panels).*

3 Current and volume contraction

In each experiment we considered a single very long trajectory, up to 10^{11} collisions for some low values of ε . Concerning the qualitative properties of the model, the radius r of the upper and lower sides of the cell turns out to be irrelevant, hence we present results only for $r = 2$. The half-distance d is taken to be either 0.1 or 0.2, and the radius R of the obstacle, in the closed model, is chosen midway between d and the value R_{\max} for which the obstacle grazes the sides of the cell. Unless explicitly stated, for both the open and closed model we have $\beta = \alpha^{1/2}$.

The current J is defined in the obvious way as the time average of v_x . Its behavior as function of ε is shown in figure 3, both in linear and in logarithmic scale. In this and the next figures, open and closed symbols refer respectively to the open and closed model; squares refer to $d = 0.1$ and triangles to $d = 0.2$. For given parameters, the value of J is practically independent of the particular initial datum (the difference in J is much less than the size of the symbols). A careful inspection shows that in the closed model, for low ε , the current is with very good approximation a linear function of the field,

$$J = \kappa \varepsilon ,$$

with $\kappa \simeq 0.54$ and 0.82 respectively for $d = 0.1$ and $d = 0.2$. The ratio J/ε is indeed well constant for ε smaller than, say, 0.2, see figure 4, left; correspondingly, a least-square fit on the data in logarithmic scale gives slope one, with accuracy definitely better than 1%. Concerning the open model, its behavior at first sight might appear identical, but a closer look shows it is not: indeed the lines joining the open symbols are not exactly parallel to the previous ones, and not even straight lines. An accurate investigation shows that the conductivity is not constant for $\varepsilon \rightarrow 0$, rather it exhibits a weak logarithmic divergence:

$$J/\varepsilon = \kappa_0 + \kappa_1 \log \varepsilon^{-1} ,$$

with $\kappa_0 \simeq 0.20$, $\kappa_1 \simeq 0.87 \times 10^{-2}$, for $d = 0.1$; see figure 4, right. The logarithmic correction is likely related to the presence of the straight horizontal trajectory, whose positive Lyapunov exponent tends to zero for decreasing ε , and for small ε opens the horizon. We did not investigate further this point.

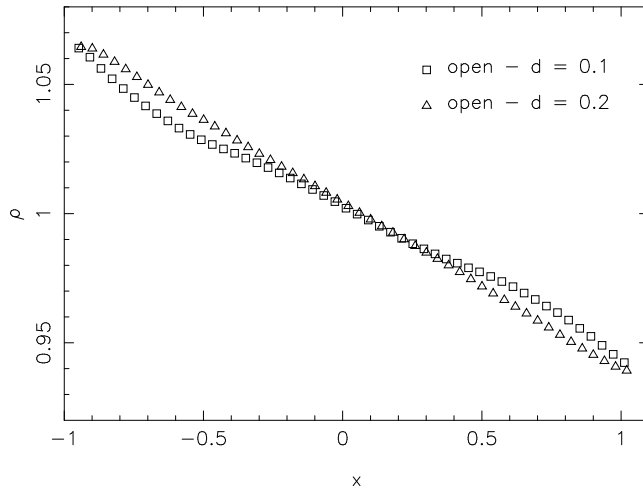


Figure 5: *The density profile, for the open model.*

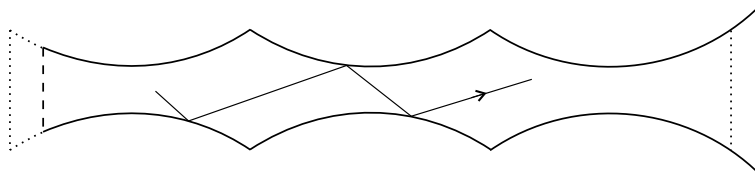


Figure 6: *The potential difference is applied every L cells ($L = 3$, here).*

It is also possible to define a density $\rho(x)$ of the gas in the cell, dividing the cell into a large number of thin vertical strips, and posing $\rho_j = t_j/(TS_j)$, where t_j is the time spent by the particle in the j -th strip up to the total time T , and S_j is the area of the strip. Relying on the likely ergodicity of our system, ρ_j is taken as an approximation of the density of particles in the midpoint x_j of the strip. The result, for the open model at $\varepsilon = 0.1$, is exhibited in figure 5. The impression is that ρ is a smooth decreasing function of x , interpolating the densities of the left and right reservoirs (there is no reason for this curve to be linear).

As remarked above, as far as the length of the model is fixed, it is not possible to distinguish between field and potential difference. To show that ε has the properties of a potential difference applied at the ends of the cell, and to check that J is driven by the corresponding field, we introduced models of different lengths, applying the same asymmetry of size ε at the ends of sequences of L cells, with variable L , cf. figure 6. We then tested whether the resulting current was inversely proportional to L or not. Let us remark that, according to the law of gases, the pressure difference is, up to a multiplicative constant, $1/|\Sigma^-| - 1/|\Sigma^+|$, and in turn this is proportional to $\alpha - 1 \simeq \varepsilon$; normal transport then requires the current to be proportional to ε/L . The result of our calculations is reported in figure 7, where J is plotted vs. L in logarithmic scale, for the open model, for two values of ε and two values of d , in the interval $1 \leq L \leq 12$. The data are well fitted by straight lines, and the slope of all of them turns out to be -1 , with accuracy better than 1%. The conclusion is that, in this one respect, the transport looks normal.

As far as dissipation is concerned, we observe that collisions with the reflecting walls preserve the volume of the phase space, so that the Jacobian \mathcal{J}_i for the i -th collision along a given trajectory is 1. Collisions with Σ^\pm , instead, introduce a dissipation determined by $\mathcal{J}_i = \mathcal{J}^\pm$,

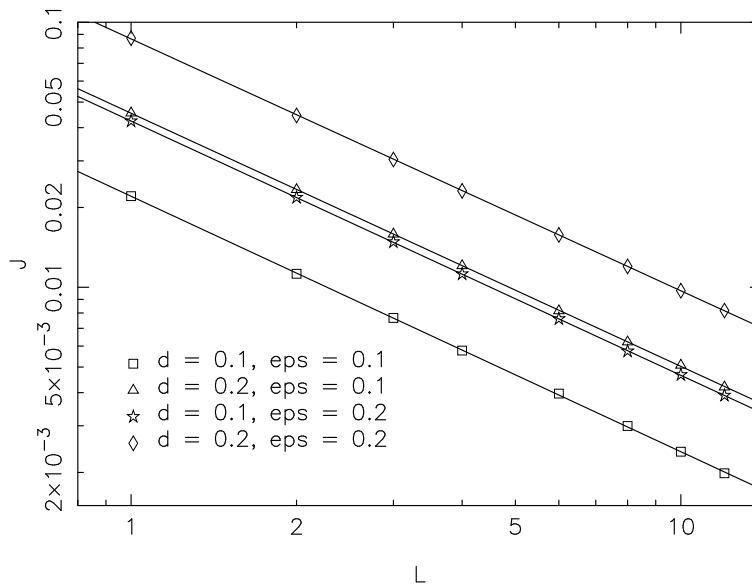


Figure 7: *The current J vs. the number L of cells.*

with \mathcal{J}^\pm given by (3). The Lyapunov exponent χ_v of the volume (normalized to the number of collisions) is then given by

$$\chi_v = \lim_{n \rightarrow \infty} \chi_v^{(n)}, \quad \chi_v^{(n)} = \frac{1}{n} \sum_{i=1}^n \log \mathcal{J}_i.$$

Thanks to the large number of collisions we were able to compute, it was possible to determine the limit χ_v with good accuracy; in typical cases, we observed that $\chi_v^{(n)}$ was well stable, with residual oscillations not exceeding (and frequently less than) 1%, for n between the final value and one quarter or even one tenth of it.

Figure 8a reports $-\chi_v$ vs. ε , in logarithmic scale, both for the open and the closed model, each for two different values of d (lower curves, along the diagonal). For small ε , χ_v appears to be proportional to ε^2 . More precisely, for the closed model and $\varepsilon \leq 0.2$, say, our data are well interpolated by straight lines of slope 2, with accuracy better than 1%. For the open model instead χ_v has, similarly to J , a logarithmic correction. In fact a closer analysis shows that in all cases, for small ε , χ_v is proportional to the product εJ , the ratio $\chi_v/(\varepsilon J)$ being divergence free; see figure 8b.

Let us stress that, while in Gaussian thermostatted systems the proportionality of χ_v to the product εJ is guaranteed [CR98], and remains valid at large ε too, instead in our model such a proportionality is not obvious, and in fact it is lost at large fields. Assuming this proportionality holds also for systems of interacting particles subjected to the same field and thermostat considered here, we have an intriguing connection between purely dynamical quantities and thermodynamic quantities. In that case, indeed, ε and J can be identified with a thermodynamic force and a thermodynamic flux, respectively, hence at small ε the phase space contraction rate is proportional to the “entropy production rate” εJ . Let us also observe that the loss of proportionality that we find at large fields is consistent with the fact that the entropy production rate is no more expected to be quadratic in the field for large fields. In this one respect, our model of a thermostat looks more realistic than the Gaussian thermostat.

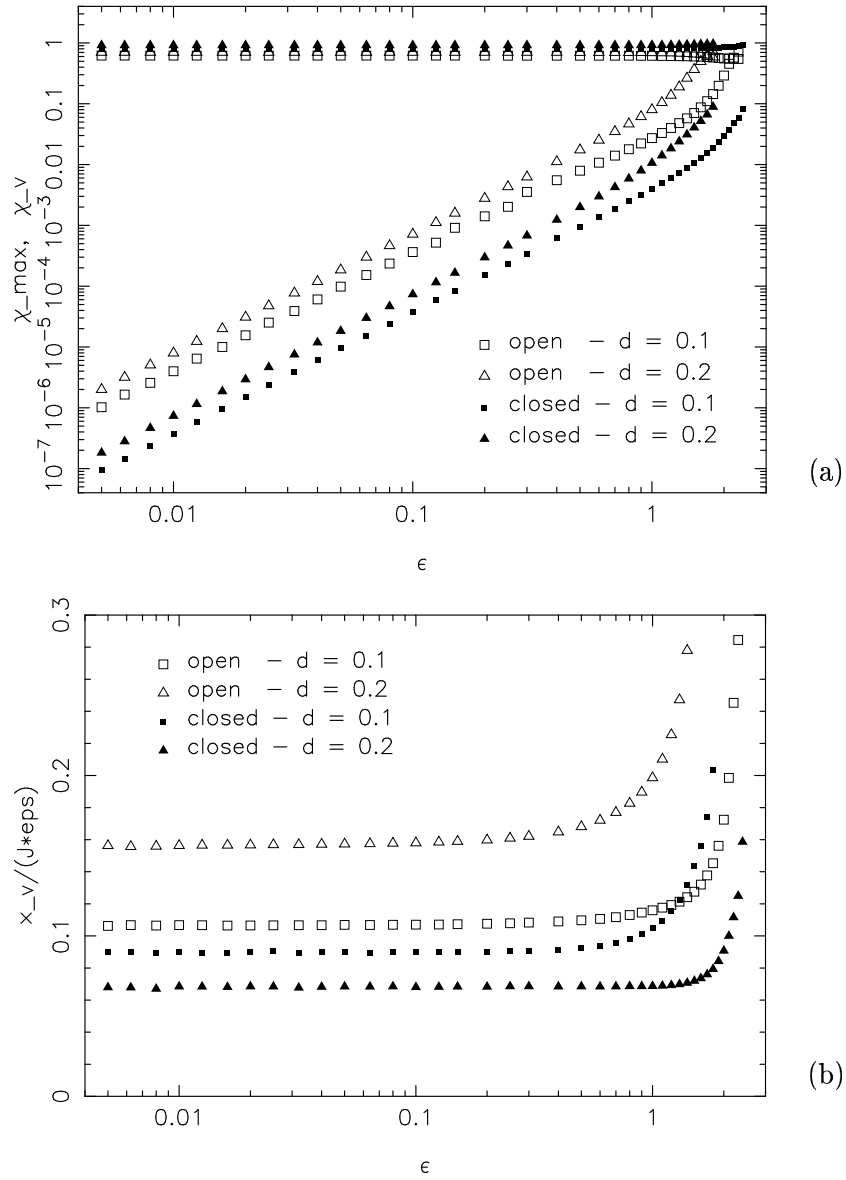


Figure 8: (a) The Lyapunov exponents χ_{\max} (upper horizontal curves) and $-\chi_v$ (lower curves), as functions of ϵ , in logarithmic scale; (b) the ratio $-\chi_v / (\epsilon J)$.

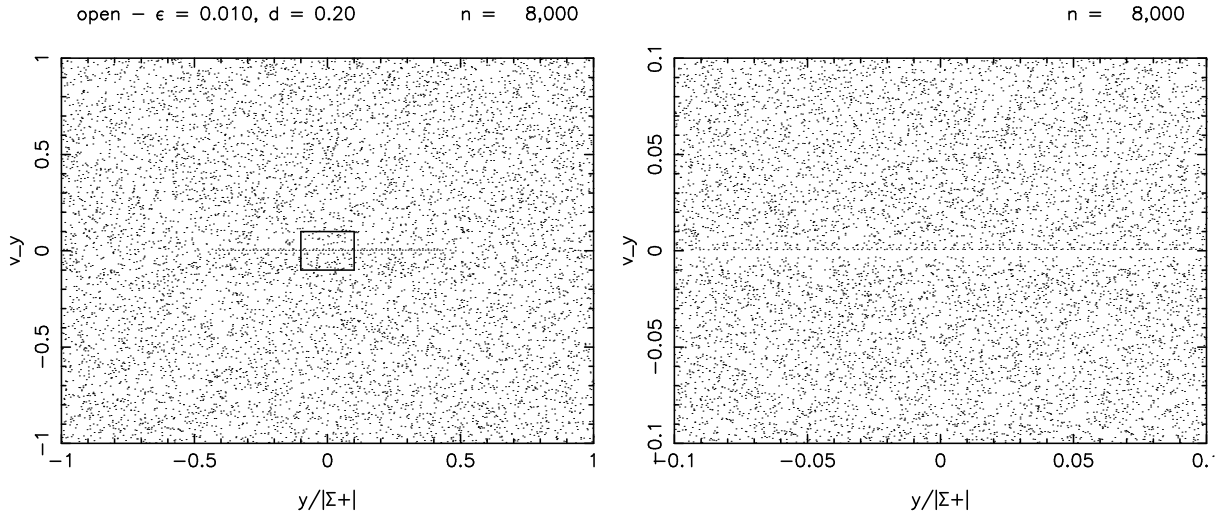


Figure 9: *The Poincaré section for the open model, $d = 0.2$, $\varepsilon = 0.01$.*

For the sake of completeness, we also computed the maximal Lyapunov exponent χ_{\max} of the billiard map. The result is reported in figure 8a (upper, nearly horizontal curves). Not surprisingly, for a given geometry and for $\varepsilon \rightarrow 0$ (hence also $\beta \rightarrow 0$), χ_{\max} tends to a nonvanishing limit.

4 On the invariant measure

Let us consider the Poincaré section corresponding to “collisions” with Σ^+ . Each collision is naturally described by two coordinates $\tilde{y} = 2y/|\Sigma^+|$ and v_y , $(\tilde{y}, v_y) \in \Lambda = [-1, 1]^2$; the Poincaré map $\Phi : \Lambda \rightarrow \Lambda$ associates to each collision the next collision. For $\varepsilon = 0$, the Lebesgue measure $d\mu_0 = d\tilde{y} dv_y$ on Λ is preserved by Φ , and correspondingly, the system being ergodic, almost all trajectories uniformly fill Λ . For small positive ε , the CH states that the system should behave as a transitive Anosov system, whose typical trajectories densely explore all regions of Λ with a frequency given by a SRB measure $d\mu_\varepsilon$, singular with respect to $d\mu_0$.

Figures 9-11 show the Poincaré section for the open model with $d = 0.2$, for different values of ε . For graphical reasons, the number of points in each panel is limited to 40,000. Points are produced as consecutive iterations of the map, after some transient. Figure 9 refers to $\varepsilon = 10^{-2}$; for such a small field the dissipation is very small, and the distribution looks uniform; zooming in the central rectangle, see the right panel, still reveals a uniform distribution (with the possible exception of a thin line at $v_y = 0$, very likely due to the slow decay of correlations around the weakly unstable horizontal collisionless trajectory). For growing ε , instead, some structure gets progressively more evident. For example, figure 10 refers to $\varepsilon = 0.5$, and shows that the invariant measure is nontrivial and has a selfsimilar structure. The same structure can be observed for smaller values of ε , too, although by decreasing ε it becomes less and less evident; indeed some structure ought to exist for any positive ε , because in that case the uniform distribution is not invariant under the iterations of the map. For larger ε , the system visibly fails to be transitive: in Λ there appear empty regions, that is regions of positive Lebesgue measure but zero physical measure. For still larger ε , the support of the measure collapses onto a self-similar attractor of zero Lebesgue measure; see, for $\varepsilon = 1.8$ (the largest value of ε compatible with the geometry of

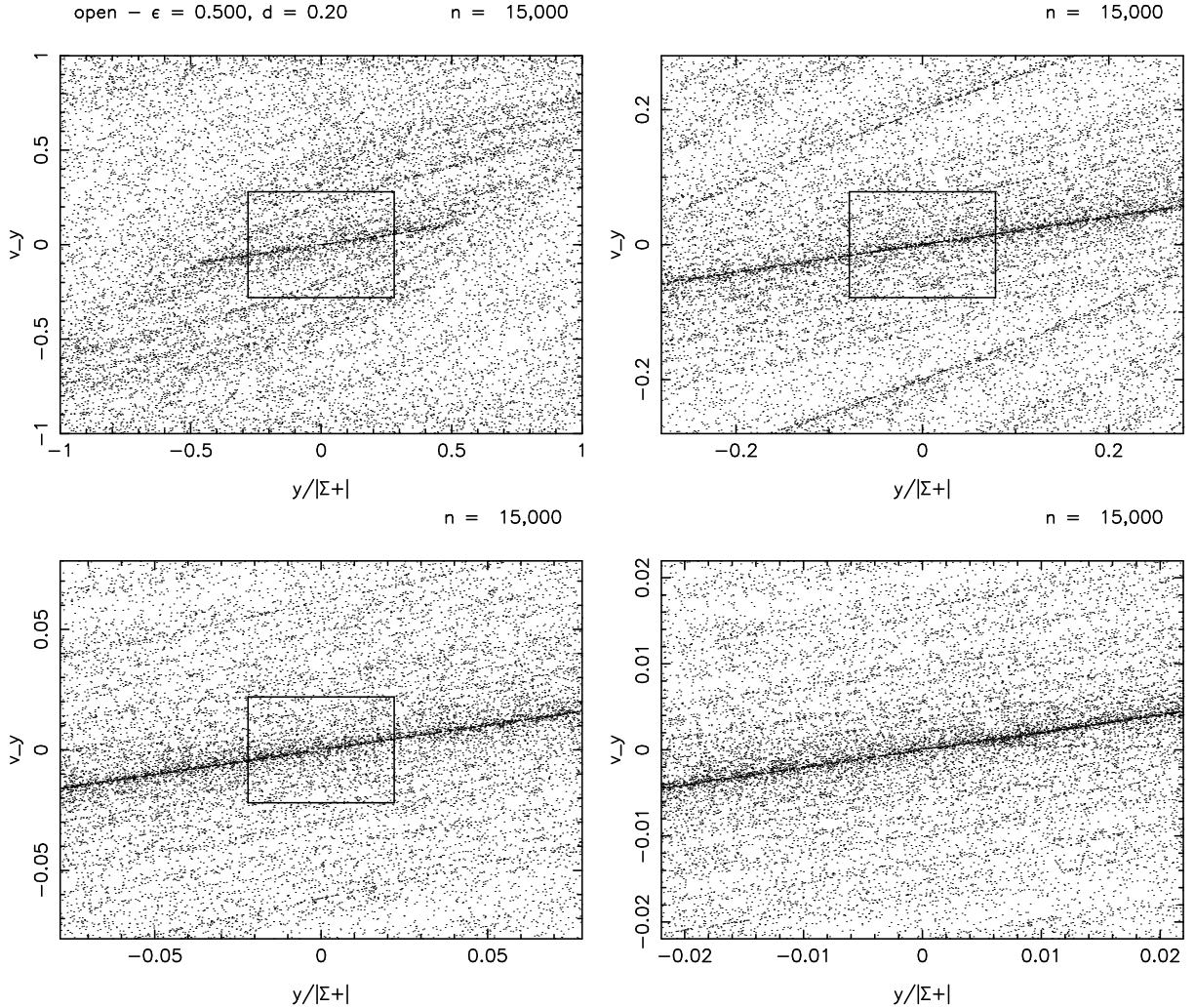


Figure 10: *The Poincaré section for the open model, $d = 0.2$, $\varepsilon = 0.5$.*

the model at $d = 0.2$), figure 11.

The closed model behaves somewhat differently: the phase space distribution looks uniform to the eye up to $\varepsilon = 1.5$, and even beyond that value (which is very large), the lack of uniformity is not as sharp as in the open model. In particular, the self-similar structure is not evident in the phase space distribution of the closed model.

5 The fluctuation formula

We made an effort to test, in our model, the Gallavotti–Cohen fluctuation formula [GC95], concerning the fluctuations of the dissipation rate. Such a formula — a sharp one, with no free constants — plays a crucial role in the theory proposed by these authors. In particular, the formula constitutes the first result derived within this framework, and leads to the Onsager reciprocal relations in the limit of small driving fields. The test we performed follows very closely the one described in [BGG97], and similarly it shows that the fluctuation formula is satisfied by our models within quite small error bars. An interesting difference, however, is

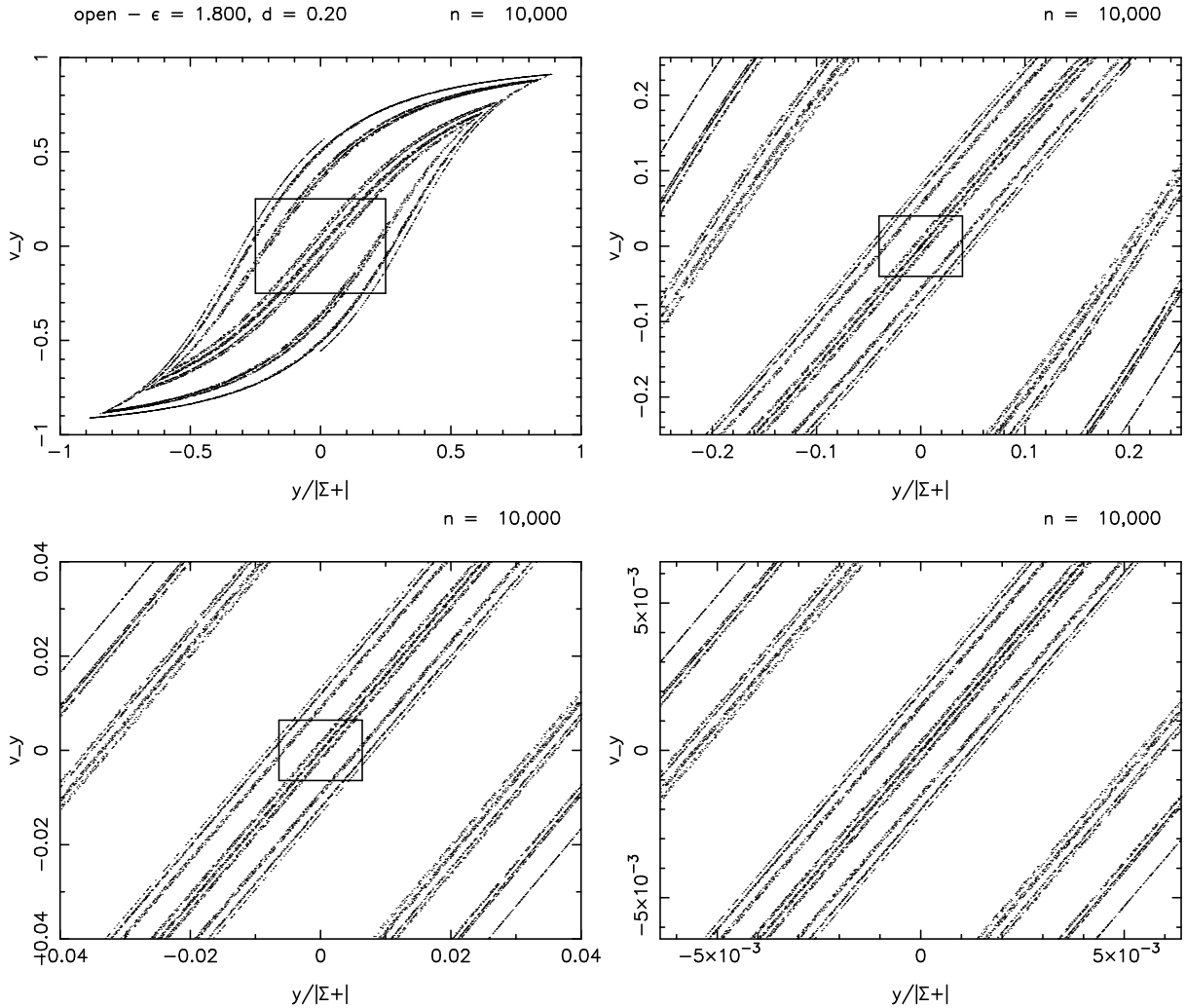


Figure 11: *The Poincaré section for the open model, $d = 0.2$, $\varepsilon = 1.8$.*

that *the fluctuations of our open model are manifestly not Gaussian*, similarly to the cases, e.g., of Refs.[LLP98,RM01]. This fact clearly shows the difference between the Gallavotti–Cohen Fluctuation Theorem, which is a large deviations result, and the Central Limit Theorem, which is verified by the small fluctuations of chaotic systems.¹

Consider a long trajectory, with a total number n of collisions with any of the cell sides, including crossings with Σ^\pm , and divide it into m segments of N collisions, separated by intervals of N_0 collisions, so that $n = m(N + N_0)$. Let λ_j denote the “finite time Lyapunov exponent” of the volume, normalized to the time:

$$\lambda_j = -\frac{1}{\tau_j} \sum_{i=(j-1)(N+N_0)+1}^{j(N+N_0)} \log \mathcal{J}_i ,$$

¹Large fluctuation can of course also *look* Gaussian, as in [BGG97] and, see below, in our closed model, but cannot really be Gaussian in these models, because they take values in a bounded interval.

where τ_j denotes the time length of the j -th segment, and denote

$$\langle \lambda \rangle = \frac{\sum_{j=1}^m \tau_j \lambda_j}{\sum_{j=1}^m \tau_j}, \quad p_j = \frac{\lambda_j}{\langle \lambda \rangle},$$

which yields $\langle p \rangle = 1$ for the average of p . Let π be the distribution law of the values p_j . The Gallavotti–Cohen fluctuation formula states that in the limit of long segments, i.e. for large N , the distribution π obeys the law

$$\log \frac{\pi(p)}{\pi(-p)} = \langle \lambda \rangle \langle \tau \rangle p.$$

In practice, one compares

$$\xi = \frac{1}{\langle \lambda \rangle \langle \tau \rangle} \log \frac{\pi(p)}{\pi(-p)}$$

with p , for larger and larger N . Concerning N_0 , the only prescription is that it be sufficiently large, so that nearby segments result uncorrelated, and the corresponding values λ_j independent. We used $N_0 = 100$ collisions or larger, and N up to 4000. The test of the fluctuation formula must be quantitative, since there are no free parameters that can be adjusted to match a qualitative correspondence, so error bars are required. We produced them using the rule of the three standard deviations, as done in Ref.[BGG97].

A typical result for the closed model is produced in figure 12. The figure refers to $\varepsilon = 0.125$, $d = 0.1$; the left panels reproduce the distribution π , for $N = 200, 1000$ and 4000 (top to bottom), while in the corresponding right panels the numerical results for ξ are compared with the theoretical expectation $\xi = p$ (the line). The statistics is rather large: for $N = 4000$ the total number of segments is $m = 2 \times 10^7$ (with $N_0 = 1000$, it is $n = 10^{11}$), and correspondingly the error bars are rather short. The fluctuation formula appears to be well satisfied up to, at least, $p = 10$, to be compared with the standard deviation $\sigma \simeq 2.9$ of π , $\sigma^2 = \langle (p-1)^2 \rangle$. Figure 13 shows the corresponding quantities for $\varepsilon = 0.5$ and same values of N . The formula is well satisfied up to $p=1.6$. The corresponding fluctuations are remarkably large: the distance of $-p$ from $\langle p \rangle = 1$ extends to 2.6, to be compared with $\sigma \simeq 0.50$. Concerning the shape of π , in all tests we made on the closed model, we found that π is indistinguishable from a Gaussian. In particular the kurtosis $k = \langle (p-1)^4 \rangle / \langle (p-1)^2 \rangle - 3$ is very small, i.e. of the order 10^{-3} for large N , and moreover it decreases with N approximately as N^{-1} , as in [BGG97]. For example, in the case of figure 12 it is $k = -3.0 \times 10^{-2}$, -8.6×10^{-3} and -2.4×10^{-3} respectively for $N = 200, 1000$ and 4000 .

The situation is different for the open model, as is shown in figure 14 for $d = 0.1$ and $\varepsilon = 0.1$. The figure refers to the same values of N , and reports the same quantities as figures 12 and 13. The distribution π , however, is reported in logarithmic scale, to make evident even at first sight that the distribution is not Gaussian (the curve visibly deviates from a parabola, and is not even symmetric). Correspondingly, the kurtosis is large: for the above values of N we found, in the order, $k = 0.67, 1.17$ and 0.61 . In spite of this, the fluctuation formula appears to be well satisfied, actually equally well as for the closed model. The next figure 15 refers to $\varepsilon = 0.02$, and shows an even more striking deviation from the Gaussian; the kurtosis for $N = 4000$ is now $k \simeq 4.6$. Very likely, the non Gaussian behavior observed in this case is related to the open horizon and to the correspondingly slow correlations decay as, indeed, the effect is larger for smaller ε , i.e. when the horizontal orbit is less unstable. However, we have not found a definite

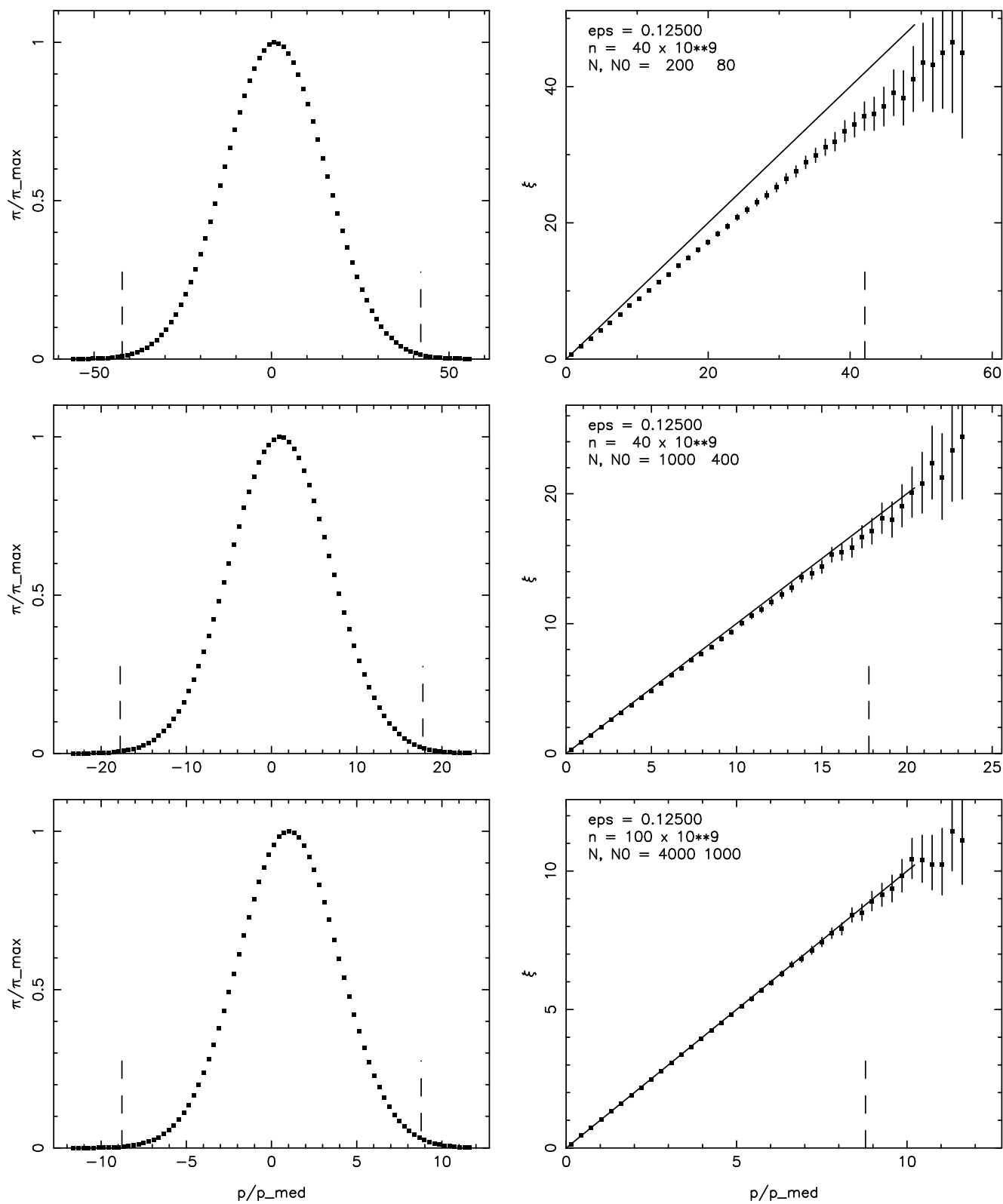


Figure 12: Closed model, $d = 0.1$, $\varepsilon = 0.125$: the distribution π for $N = 200$, 1000 and 4000 (left, top to bottom); the corresponding numerical data for ξ , compared to the theoretical expectation $\xi = p$ (right).

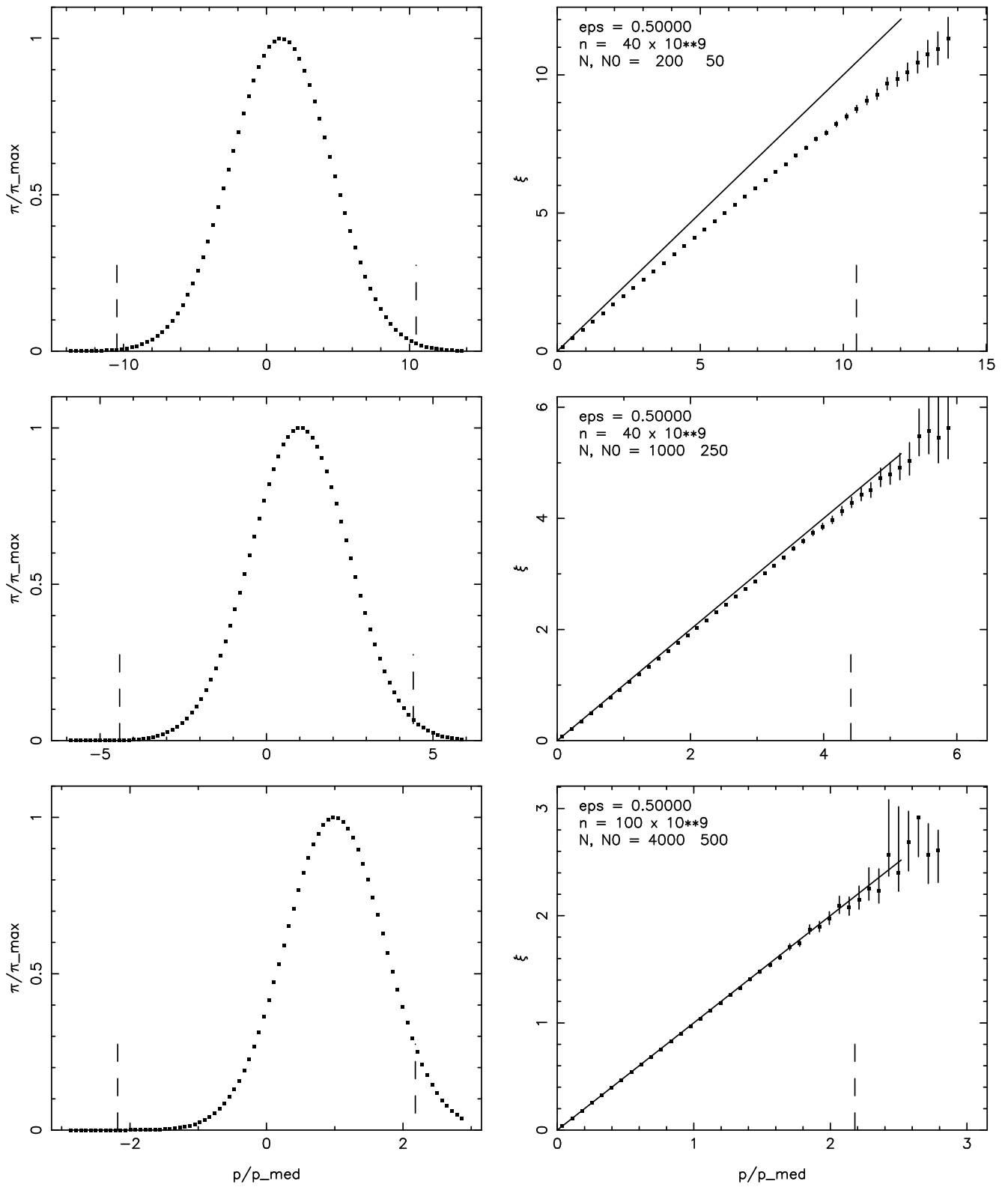


Figure 13: Same as figure 12, for $\varepsilon = 0.5$

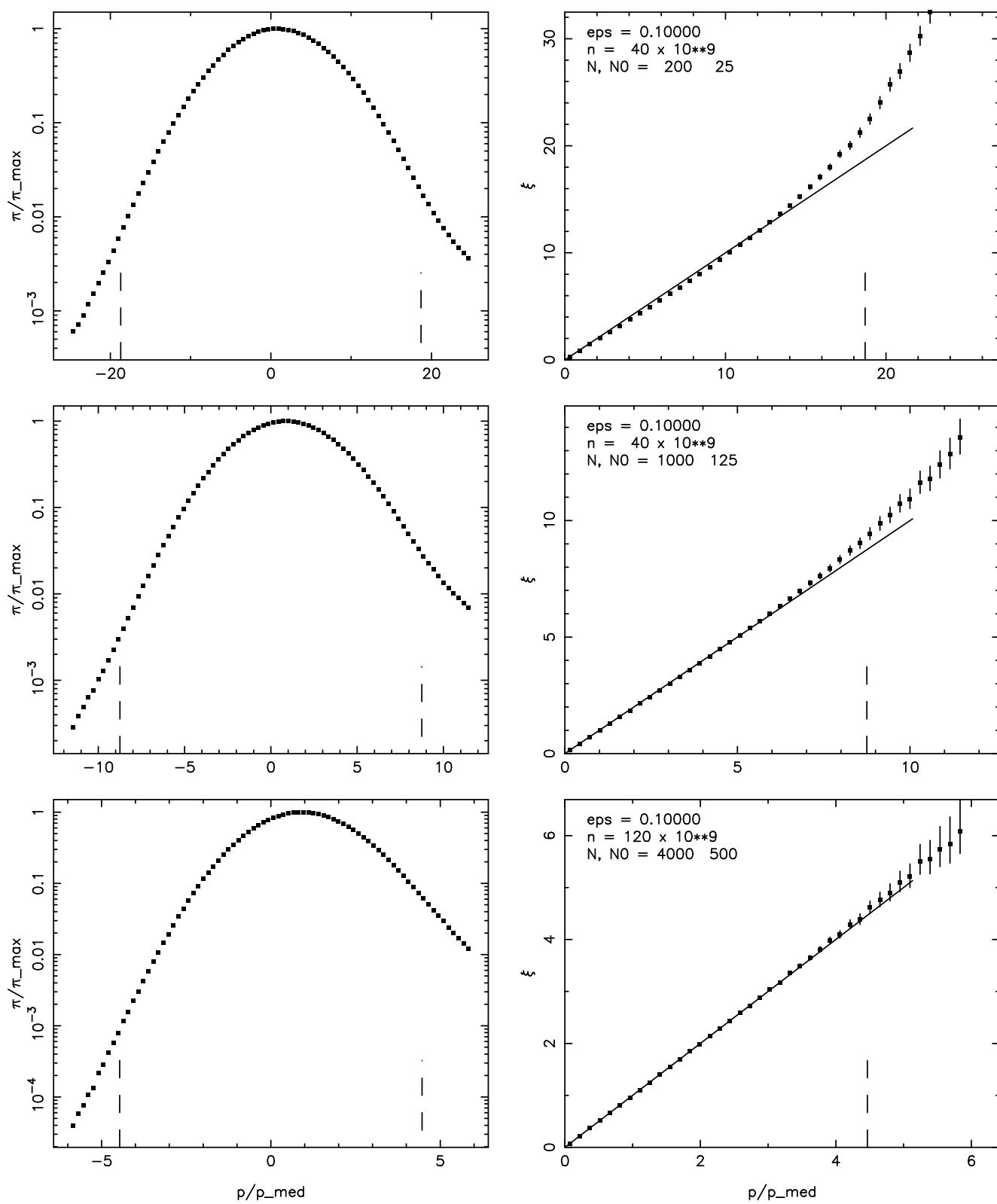


Figure 14: Same as figures 12 and 13, for the open model, at $d = 0.1$, $\varepsilon = 0.1$.

link between the non-Gaussianity of π , which is a symptom (a definition, in some context) of intermittent behaviour, and the decay of correlations.²

6 Further experiments, and concluding remarks.

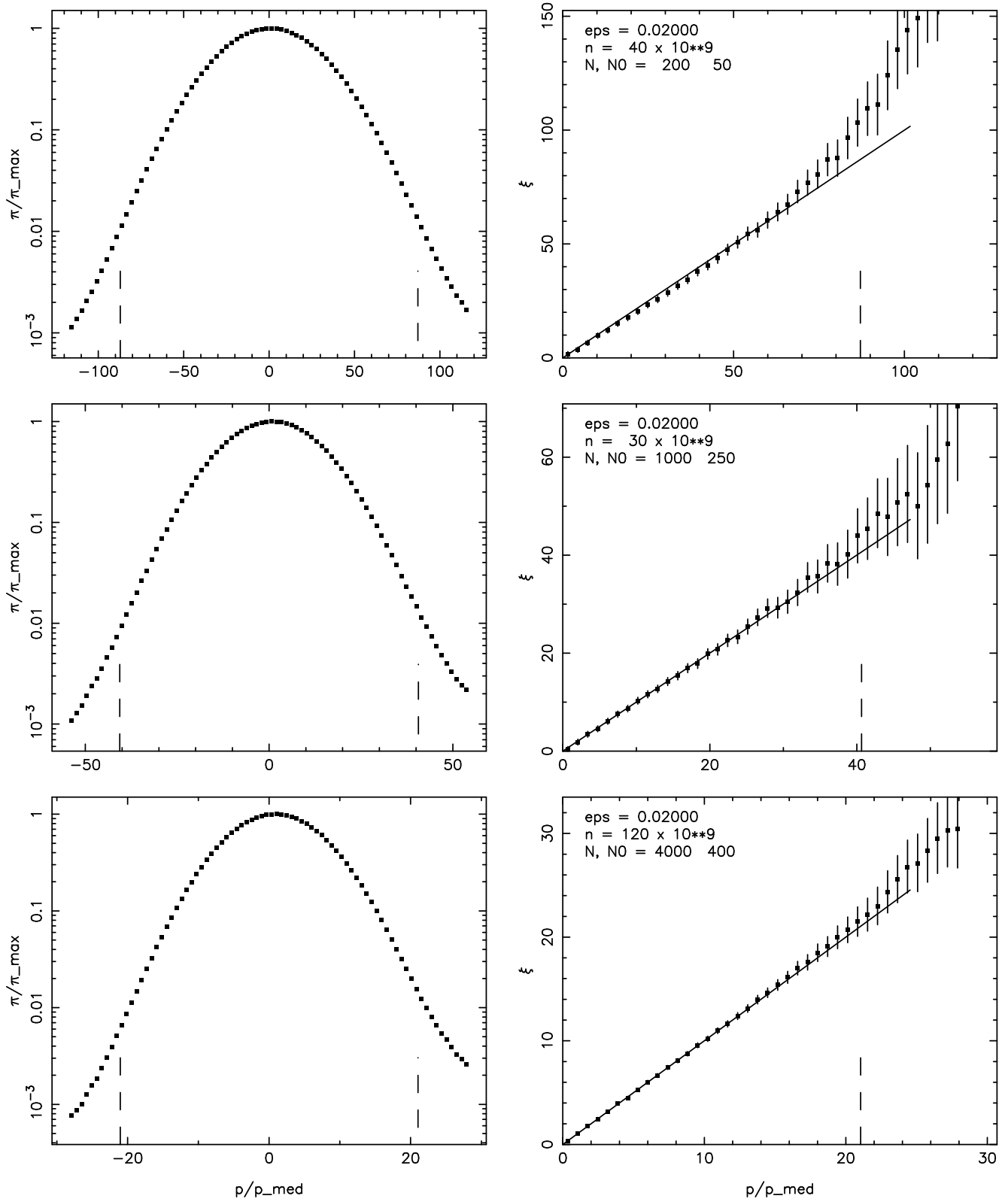
A. Flat sides. As remarked in the Introduction, one of the purposes of this paper is to understand how far one can simplify the microscopic dynamics, still obtaining (formally, at least) a normal transport process. Figure 16 shows a model similar to the open one, but differing from it in a relevant point: the reflecting sides of the cell are now flat, and correspondingly the zero field model, as any polygonal billiard, is not hyperbolic, though, for suitable geometry, the system can be made ergodic [GU96]. Hyperbolicity is an essential feature of the Gallavotti–Cohen theory, and in complete lack of it one could think that the CH is not justified. However, a study of transport phenomena in a flat billiard with a small electric field [LRB00] revealed that decreasing the field there are longer and longer transients during which the behavior of the system looks rather similar to that of a chaotic steady state, despite the fact that the asymptotic evolution is trivial: all trajectories collapse onto periodic (up to lattice translations) orbits. Therefore, the validity of the fluctuation formula, properly interpreted, could be established in the limit of small fields.

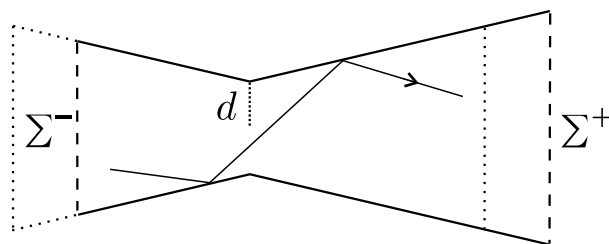
We considered the model of figure 16, with reflecting sides forming angles φ and $\pi - \varphi$ with the x axis; for $\varepsilon = 0$ the end sides Σ^\pm are at ± 1 , while for $\varepsilon > 0$ they are moved of the same amount to the right, till $\alpha = |\Sigma^+|/|\Sigma^-| = \exp \varepsilon$. After some trials, we chose $\varphi = 0.51\pi/(2\sqrt{2})$.

The results we obtained are similar to those of Ref.[LRB00], but sharper thanks to better statistics. More precisely:

- i. In all cases we observed a collapse onto a periodic orbit but, differently from [LRB00], with vanishing current. The period depends very irregularly on ε , and is often very large; for example, for $d = 0.1$ and $\varepsilon = 0.2$ the attracting periodic orbit closes after 434 collisions. The transient before the collapse is irregular as well, and can be very long: it is frequently between 10^6 and 10^7 of collisions, and occasionally (in particular, for the above orbit of period 434) it gets larger than 10^9 collisions.
- ii. The periodic orbits are only marginally attractive: their maximal Lyapunov exponent χ_{\max} is zero within our precision, i.e. $|\chi_{\max}| < 10^{-9}$. The volume exponent χ_v is instead definitely negative ($\chi_v \simeq -7.5776 \times 10^{-4}$, for the above long periodic orbit) and thanks to periodicity, the result is very accurate.
- iii. During the transient, especially if long, the behavior of the system looks similar to a normal transport process. In particular, the current is positive; the Poincaré section shows an almost uniform distribution, as if there were an invariant measure with support on Λ ; χ_{\max} and χ_v approach respectively a positive and a negative value (the latter being different from the asymptotic one). Concerning the fluctuation formula, the result for $d = 0.1$, $\varepsilon = 0.2$ and a transient of 1.3×10^9 collisions is shown in figure 17. The impression is that the formula is still satisfied for all N compatible with the length of the transient, though not as well as in the hyperbolic cases. The distribution π is visibly non Gaussian.

²Further computations for $\varepsilon = 0.1$ and $N = 8000$ (though with less statistics) give $k = 0.36$, suggesting that for asymptotically large N the kurtosis might decrease to zero in the open model, too. The point however is that the fluctuation formula is very well satisfied also for k of order one.

Figure 15: Same as figure 14, for $\varepsilon = 0.02$.

Figure 16: *The flat model.*

According to a nice sentence³ by Einstein: “*Everything should be made as simple as possible, but not simpler.*” It seems that here, as in [LRB00], we are locating one piece of the borderline between “simple” and “simpler”.

B. The role of β . As remarked in Section 2, for the closed model the choice of β is not as crucial as for the open model, and the elementary re-injection law $\beta = 1$ also gives rise to a nontrivial dynamics. However, $\beta = 1$ is not well suited for testing the fluctuation formula: indeed for $\beta = 1$ it is $\log \mathcal{J}^\pm = \mp \varepsilon$, and for each segment of trajectory the quantity $\sum_i \log \mathcal{J}_i$ is a multiple of ε . Since for large N the time τ_j is also nearly constant, namely nearly equal to $N\langle\tau\rangle$, the result is that p is a discrete variable, appearing in multiples of $\varepsilon/(N\langle\tau\rangle)$. Though for increasing N such a quantity gets smaller, and correspondingly π approaches a continuous distribution, for the N achievable in practice, the presence of the discontinuities is rather evident.

What is easy, anyhow, is looking at the conductivity of the closed model for different values of β . Figure 18 (left) shows J as function of ε , for $\beta = 1$, $\beta = \sqrt{\alpha}$ and $\beta = \alpha$, in the linearity interval $0 < \varepsilon \leq 0.2$. The conductivity falls practically to zero for $\beta = \alpha$, while for $\beta = 1$ it is higher than for $\beta = \sqrt{\alpha}$. A closer inspection shows that the conductivity J/ε is exactly proportional to δ , if δ is such that $\beta = \alpha^{1-\delta}$; see figure 18 (right).

C. Concluding remarks.

It is interesting to note that our models of noninteracting particles seem to give rise to transport processes described by the usual laws of IT, although the mechanisms which are at work in our models are rather different from those of the systems considered in IT [CR01].

How is it possible that relations formally identical to Ohm’s law, Fick’s law etc, can be obtained for systems such as ours? Our analysis suggests that the chaoticity of the motion, coupled to the presence of the “thermostat” introduces some kind of dissipation in the dynamics of our systems, that gives rise to formally normal transport. As a matter of fact, we noticed logarithmic corrections to the linear laws in the case of infinite horizon, which is less chaotic than the closed model. Moreover, differently from IT, in that case, the deviations from the linear laws remain even when the fields are reduced. At the same time, we noticed that as long as the dynamics is sufficiently complex, although not really chaotic, like in the case of flat billiards, the transport process looks normal.

It seems then that a certain degree of chaoticity and dissipation is at the basis of the linear laws, as well as of the fluctuation formula. In real systems this chaoticity and dissipation is mainly due to the interactions of the particles with themselves and with their environment, while in noninteracting models the geometry and the “thermostats” are responsible for the chaoticity and the dissipation.

³Quoted in: G. Iooss and D.D. Joseph, *Elementary Stability and Bifurcation Theory*, Springer, New York 1980.

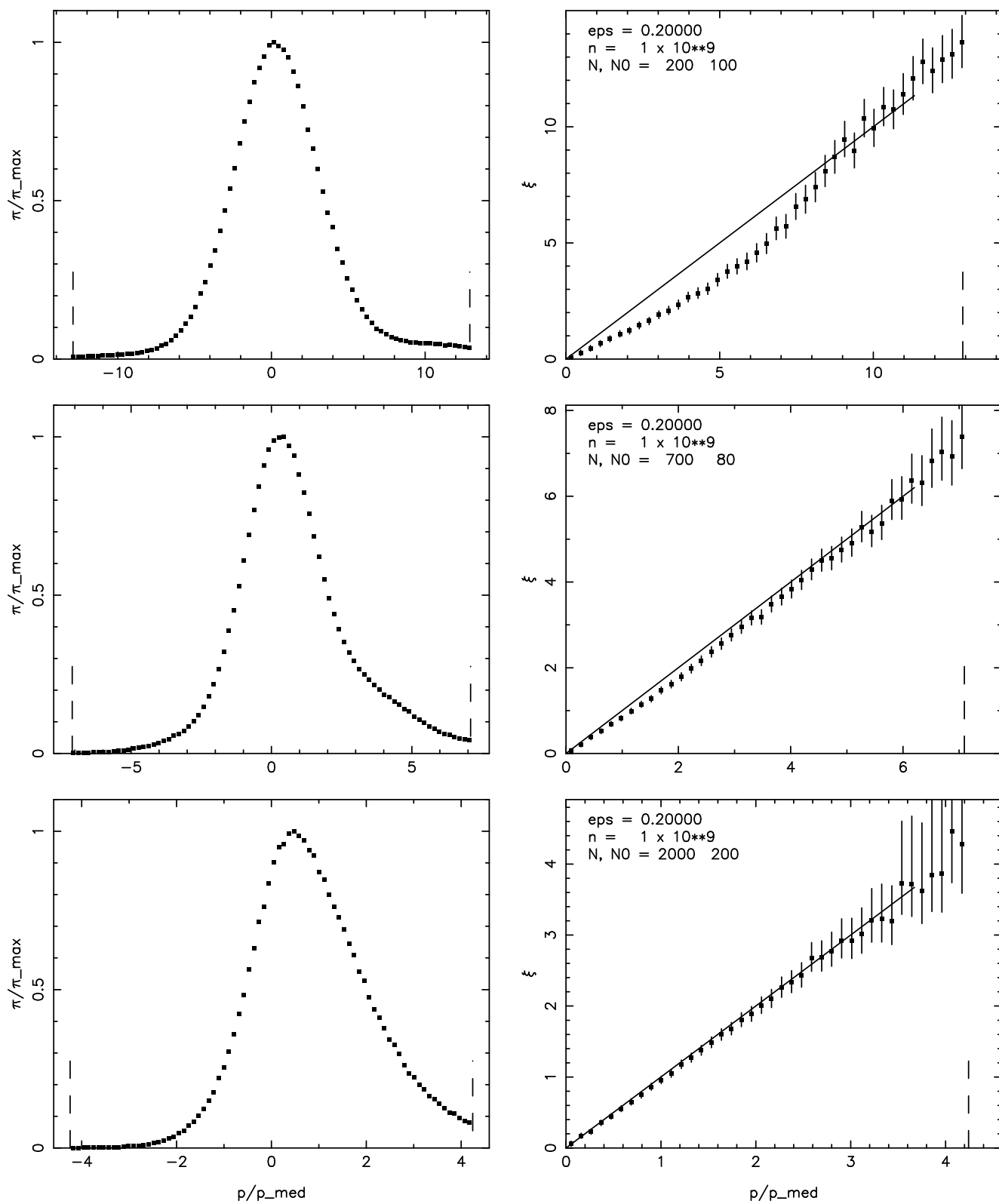


Figure 17: Flat model, $d = 0.1$, $\varepsilon = 0.2$: the distribution π for $N = 200$, 700 and 2000 (left, top to bottom); the corresponding numerical data for ξ , compared to the theoretical expectation $\xi = p$ (right).

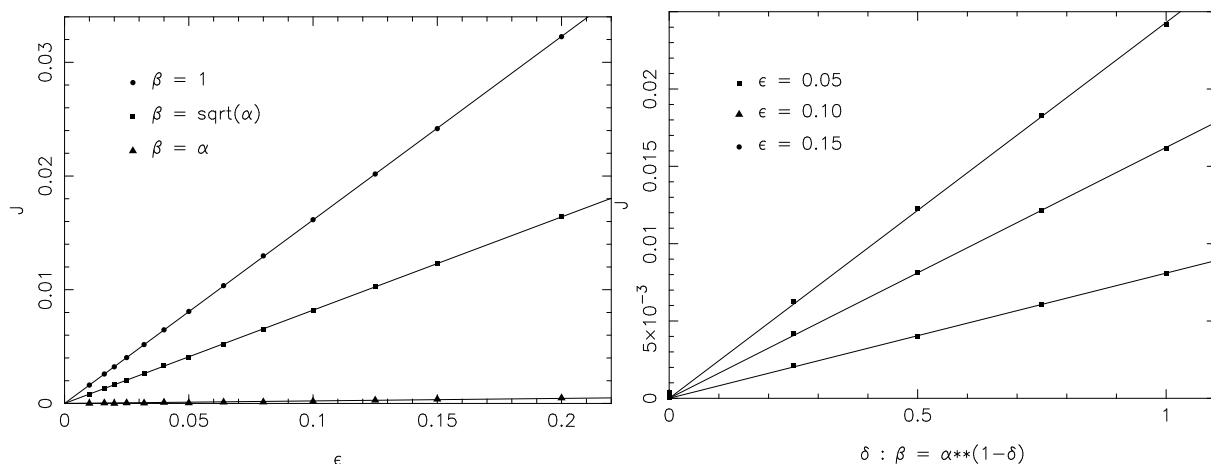


Figure 18: J as function of ϵ , for three choices of β , for the closed model with $d = 0.2$ (left); J as function of δ , for three choices of ϵ , same model (right).

In particular, our models with $\beta = 1$ have a dissipation which coincides with the entropy production of an isothermal compression of an ideal gas. The situation is less clear for the cases with $\beta \neq 1$. The meaning of these facts requires further investigation, which will be the subject of future works. Other open questions which will be studied in the future concern: 1) the hyperbolicity of our models and its consequences for the representation of the invariant measures (e.g. in terms of periodic orbit expansions); 2) the use of our “thermostat” in systems of many particles; and 3) the simultaneous presence of different driving fields, leading to cross effects and Onsager reciprocal relations.

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