On the Validity of the Conjugate Pairing Rule for Lyapunov Exponents

F. Bonetto[†], E.G.D. Cohen[‡], C. Pugh[*]

Abstact: For Hamiltonian systems subject to an external potential, which in the presence of a thermostat will reach a nonequilibrium stationary state, Dettmann and Morriss[1] *proved a strong conjugate pairing rule (SCPR) for pairs of Lyapunov exponents in the case of isokinetic (IK) stationary states which have a given kinetic energy. This SCPR holds for all initial phases of the system, all times t and all numbers of particles N. This proof was generalized by Wojtkovski and Liverani*[2] *to include hard interparticle potentials. A geometrical reformulation of those results is presented. The present paper proves numerically, using periodic orbits for the Lorentz gas, that SCPR cannot hold for isoenergetic (IE) stationary states, which have a given total internal energy. In that case strong evidence is obtained for CPR to hold for large N and t, where it can be conjectured that the larger N, the smaller t will be. This suffices for statistical mechanics.*

Keywords: dynamical systems, Lyapunov exponents, symmetry, pairing rule.

1. Introduction.

This paper consists of three parts: a statistical mechanical, a numerical and a mathematical part. They are not equally accessible to readers interested in the new and developing interaction between dynamical systems theory and statistical mechanics of dissipative systems. This reflects, in our opinion, the multidisciplinary approach involving on the one hand the mathematical theory of dynamical systems and on the other hand the physical theory of dissipative macroscopic, *i.e.* , statistical mechanical systems. In order to make progress towards a deeper understanding of the dynamical foundation of the statistical mechanics of dissipative macroscopic systems, such a combined approach seems unavoidable. However, it leads, regrettably, to difficulties in understanding the language of the different disciplines.

Since this paper is primarily adressed to physicists, we have written the core of the paper in a language that should be accessible to a large portion of them. However, an interesting

[†]Rockefeller University. Present address: Mathematics Department, Rutgers University

[‡]Rockefeller University

[*]Mathematics Department University of California Berkeley California, 94720

mathematical unification and reformulation of previous results has been obtained by one of us (C.P.). This work is of a more mathematical nature than the rest of the paper, but make a connection between mathematics and physics, in particular the mathematics of symplectic spaces and the physics of thermostatted dynamical systems. For that reason we have summarized the main results of this work in a Discussion Remark, but reserved a sketch of the details to an Appendix.

The modelling of dissipative macroscopic systems by dynamical systems, i.e., by sets of equations of motion for the particles of the system, which mimic the behavior of such systems under the influence of an external field in a nonequilibrium stationary state, can be achieved by adding a suitable dynamical thermostatting term to the equations of motion. In fact, in all computer simulations the dynamical system reaches a stationary state, by adjusting a thermostat term in the equations of motion in such a way that the heat developed due to the work done on the system by the external forces is removed via effective friction terms in the equations of motion of the system. This approach has raised a lot of interest in the last ten years. In particular in 1988, Posch and Hoover[3] found a relationship between the average phase space contraction rate of a many particle color diffusion system under the influence of an external color field and the work done on the particles of the system, if the internal energy of the system in the stationary state was kept constant (iso-energetic (IE) thermostat). Another way of saying this is that in the stationary state the average phase space contraction rate of the system is equal to the irreversible entropy production rate in the system[4]. This allowed one to express transport coefficients in terms of the sum of the Lyapunov exponents of the system and established a direct relation between dynamical systems theory in phase space and macroscopic physics in ordinary space. Similar relations have been found for other dynamical systems, including those representing viscous flow, if the stationary state is one with a fixed kinetic or internal energy. In the case of hard core interparticle interactions, when no interparticle potential energy is present, iso-energetic and iso-kinetic (IK) systems, which have constant kinetic energy, are the same. Most computer experiments have been carried out for the IK case and some for the IE case as well[5],[6].

The dynamical equations describing the macroscopic systems were solved numerically, using nonequilibrium molecular dynamics (NEMD). It was found this way that an important simplification occurred - for example in the computation of the transport coefficients - in that the sum of all Lyapunov exponents, which determines the phase space contraction rate, obeys a conjugate pairing rule (CPR) (see [7]). That is, the sum of every pair of conjugate Lyapunov exponents adds up to the same (negative) constant, which is equal to the average phase space contraction rate of the system in the stationary state, which in turn was equated to the average entropy production rate of the system. Equivalently, one can say that the Lyapunov spectrum of the system is symmetric.

A mathematical proof of the CPR for the case of a possibly time-dependent, i.e., nonautonomous, Hamiltonian system with a constant friction added to the equations of motion, was given independently of the above developments in 1988 by Dressler[8]. The system she considered in this case was neither IK or IE.

For an IK Hamiltonian system consisting of N particles $i = 1, ..., N$ with a Gaussian thermostat, which keeps the kinetic energy constant[5], one has in three dimensions ($d = 3$) the Hamiltonian:

$$H(\underline{p}, \underline{q}) = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + \phi^{int}(\underline{q}) + \phi^{ext}(\underline{q}) \tag{1.1}$$

with the equations of motion

$$\begin{cases} \dot{\vec{q}}_i = \dfrac{\vec{p}_i}{m} \\ \dot{\vec{p}}_i = \vec{f}_i^{int}(\underline{q}) + \vec{f}_i^{ext}(\underline{q})) - \alpha(\underline{p}, \underline{q})\vec{p}_i \end{cases} \tag{1.2}$$

where $\alpha(\underline{p}, \underline{q}) = \alpha_{IK}(\underline{p}, \underline{q})$ is given by

$$\alpha_{IK}(\underline{p}, \underline{q}) = \frac{\sum_i \Big(\vec{p}_i, [\vec{f}_i^{int}(\underline{q}) + \vec{f}_i^{ext}(\underline{q}))]\Big)}{\sum_i \vec{p}_i^2} \tag{1.3}$$

where $\phi^{int}(\underline{q})$ and $\phi^{ext}(\underline{q})$ are the potential energy of the particles of the system and with the external field, respectively, where $\underline{p} = (\vec{p}_1, ..., \vec{p}_N)$ and $\underline{q} = (\vec{q}_1, ..., \vec{q}_N)$, $\vec{p}_i = (p_x, p_y, p_z)$ and $\vec{q}_i = (q_x, q_y, q_z)$ are three dimensional vectors, $\vec{f}_i^{int}(\underline{q}) = \partial\phi^{int}(\underline{q})/\partial\vec{q}_i$, $\vec{f}_i^{ext}(\underline{q}) = \partial\phi^{ext}(\underline{q})/\partial\vec{q}_i$, and $(\cdot, \cdot)$ represent the usual scalar product in three dimensions. $\alpha_{IK}(\underline{p}, \underline{q})$ is the thermostatting function (or effective friction) which will be determined in such a way that the total kinetic energy of the system remains constant in time. It is a mechanical representation of the heat exchange via the boundaries of the system representing the thermostat in a real system.

Dettmann and Morriss[1] recently proved a much stronger CPR than observed in the stationary states of the computer simulations: their CPR holds for every initial condition $\mathbf{x}_0 \equiv (\underline{p}_0, \underline{q}_0)$, at every time t and for any number N of particles. We refer to this Dettmann and Morriss pairing as a *strong* CPR (SCPR). Isolating two zero Lyapunov exponents, the remaining $6N - 2$ local Lyapunov exponents over time t for any initial state and any number N of particles obey the CPR. If the local Lyapunov exponents are ordered as $\lambda_1 > \lambda_2 > .... > \lambda_{6N-2}$, then adding up the conjugate pairs $\lambda_1 + \lambda_{6N-2}, \lambda_2 + \lambda_{6N-3}, ...$, leads for every such pair to a constant $- < \alpha >_t$, where $<>_t$ means a time time average of $\alpha(\underline{p}, \underline{q})$ over time t: $-\int_o^t \alpha(s)ds/t$.

It seems natural to extend the proof of Dettmann and Morriss from the IK to the IE case. The only difference is that $\alpha(\underline{p}, \underline{q})$ is not given by $\alpha_{IK}(\underline{p}, \underline{q})$ of eq.(1.3) but by the simpler expression:

$$\alpha_{IE}(\underline{p}, \underline{q}) = \frac{\sum_i (\vec{p}_i, \vec{f}_i^{ext}(\underline{q}))}{\sum_i \vec{p}_i^2} \tag{1.4}$$

We will call H_0 the constrained part of the Hamiltonian H, *i.e.*

$$H_0^{IK} = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} \tag{1.5}$$

for the IK case and

$$H_0^{IE} = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + \phi^{int}(\underline{q}) \tag{1.6}$$

for the IE case. The question then arises to what extent the Dettmann and Morriss' proof of SCPR for the equations (1.1)-(1.3) is typical for general dissipative dynamical equations.

The Dettmann and Morriss proof has recently been generalized by Wojtkowski and Liverani[2] to include hard core contributions to the interaction potential $\phi^{int}(\underline{q})$, for which $\vec{\nabla}_i\phi^{int}(q)$ is not defined.

The Dettmann and Morriss proof makes use of the observation that the CPR as stated above only holds in a 2dN-2 dimensional (i.e., a 2-co-dimensional) subspace of the full 2dN-dimensional phase space of the dynamical system. Two zero Lyapunov exponents associated with the conservation of kinetic energy and with the motion along the system's phase space trajectory have first to be eliminated, in order to allow the remaining Lyapunov exponents to pair to a different (non-zero) value. A similar procedure, replacing the conserved kinetic by the total energy does not lead to a SCPR, like that found by Dettmann and Morriss. In fact, computer simulations for the Lorentz gas indicate that, in general, no SCPR can be expected in this case. On the contrary, our computer simulations seem to indicate that the CPR may only hold for large systems and/or long times. The reason is not clear at the moment, but might be related to the special form of the friction term in eq.(1.2): $-\alpha_{IK}(\underline{p},\underline{q})\vec{p}_i$ which obtains both for Gaussian and Nosé-Hoover thermostats[5]. For, the IK condition, $\alpha_{IK}(\underline{p},\underline{q})$ contains $\phi^{int}(\underline{q})$ in addition to $\phi^{ext}(\underline{q})$ (the latter appearing exclusively in $\alpha_{IE}(\underline{p},\underline{q})$ (cf.eq.(1.4)). This could be responsible for the validity of the local CPR in the IK case. In fact, computer simulations show that the CPR continues to be obeyed to machine precision before, during and after a collision of one moving point particle interacting via a Weeks-Chandler-Andersen (WCA) potential (cf.eq.(2.1) (2.2)) with one stationary scatterer in the Lorentz gas IK case, but is violated considerably in the IE case. Although it is unclear at present why the $\alpha_{IK}(\underline{p},\underline{q})$ is able to assure the CPR, the fact that it contains $\phi^{int}(\underline{q}) = \phi^{WCA}(\underline{q})$, the same potential that causes the scattering, could well be relevant in this context. On the other hand, it is very hard to see how $\alpha_{IE}(\underline{p},\underline{q})$, which only contains the external potential, could physically force a CPR during a collision governed by $\phi^{int}(\underline{q})$.

Strictly speaking, when more than one moving particle is present in the system, the proper thermostatting condition involves, in general, the peculiar rather than the laboratory velocities, that appear in the equations (1.1)-(1.4). Especially in the case of viscous flow it is important to identify the relevant particle velocities and the temperature of the system with the peculiar rather than the actual velocities of the particles, where the former refer to the velocity of each particle relative to the average local flow velocity of the fluid at the position of the particle (cf.eqs(4.1)(4.2)). They will be used in Section 4.

Our main results can be summarized as follows.

1. For a Lorentz gas, where a single point particle moving in a regular triangular lattice of fixed spherical WCA scatterers under the influence of a (color) field subject to a Gaussian thermostat to attain a stationary state, very carefully controlled numerical simulations of period 3 to period 8 periodic orbits, have excluded the validity of strong SCPR for an IE constraint, while being consistent with an IK constraint (for all t and x_0).
2. On the other hand both IE and the use of IK with the proper thermostatting condition with peculiar, rather than laboratory velocities, for 9, 16, 32 particles moving through WCA scatterers, strongly suggested the validity of the CPR for sufficiently large N and possibly for each t, with N large enough. In fact, at present it is unclear whether $N \to \infty$ would be sufficient for the CPR to hold in general, i.e., for all t, or whether a large t condition, i.e., $t \to \infty$, should be imposed in addition.

The "mechanization" of the thermostats, as shown in the friction terms $\sim \alpha\vec{p}_i$ in the above equations, was developed in numerical simulations in the beginning of the 1980's[5]. This extended to heat exchange the "mechanization" of thermal external forces - as occur in viscous or thermal phenomena - already introduced in linear response theory in the middle 1950's[9]. Together they form a basis for a connection between statistical mechanical and dynamical systems. To what extent these "mechanized" equations of motion adequately represent the real physical systems and the application of dynamical systems theory considerations to them reflect properties of real systems, remains, at present, an open question.

For large "mechanized" systems a number of properties of real systems, such as the positivity of the entropy production[10] and the Onsager reciprocal relations[11] have recently been established. For a further discussion of this point we refer to a forthcoming paper[4].

If the generic case for the CPR to hold is large N and/or large t, then it is in general a statistical mechanical property in a nonequilibrium stationary state of a system, rather than a dynamical property, where it would hold for all N and/or all t.

The outline of the paper is as follows.

In section 2 various attempts are described to prove SCPR for the IE one particle Lorentz model, where one particle moves through scatterers placed on a regular triangular lattice. In section 3, very accurate controlled numerical results for a one particle regular IE Lorentz model are presented, which contain apparently incontrovertable evidence of a violation of the SCPR for certain periodic orbits (see Table 2), contrary to the IK Lorentz model, as proved by Dettmann and Morriss. In section 4, numerical evidence for an aymptotic CPR for large N for IE and for a different thermostat (IPK), that makes sense only for many particle systems and in which peculiar rather than laboratory velocities appear, is presented. Section 5 summarizes some of the results and their implications obtained in the paper as well as a reformulation of the strong pairing rule condition. Appendix A1 discusses the difficulties one encounters, if one tries to map an IE system into a Hamiltonian system, like is done in [12] for IK systems. Finally Appendix A2 gives a sketch of the proof of the reformulated pairing rules condition in a geometrical form.

2. Numerical results: the Lorentz model

In this and the following sections we report the numerical simulations we have done on the pairing problem. We focus our attention on the simplest system: a periodic Lorentz model with one or more moving particles through periodically arranged scatterers. The results on a single moving particle are reported in this and the next section, those on many moving particles in sec. 4.

The Lorentz model we consider in this section then consists of one particle moving in a regular triangular array of scatterers. The particle interacts with the scatterers via a Weeks-Chandler-Andersen (WCA) potential and is subject to an external field and an IK or IE thermostat. The equations of motion are thus given by eq.(1.2) where $N = 1$ and, writing direcly $\vec{q}$, $\vec{p}$ instead of $\underline{q} = (\vec{q}_1)$, $\underline{p} = (\vec{p}_1)$, we have $\phi^{ext}(\vec{q}) = (\vec{q}, \vec{E})$, with $\vec{E}$ a fixed three dimensional vector chosen to be $\vec{E} = (1.1, 0.1, 0.1)$, $\phi^{int}(\vec{q}) = \phi^{WCA}(\vec{q})$ where $\phi^{WCA}(\vec{q})$ is the (finite range) WCA potential given by

$$\phi^{WCA}(\vec{q}) = \sum_{n \in Z^3} \tilde{\phi}(\vec{q} - \vec{q}_n) \tag{2.1}$$

with

$$\tilde{\phi}(\vec{q}) = \begin{cases} \frac{1}{\|\vec{q}\|^{12}} - \frac{1}{\|\vec{q}\|^{6}} + 0.25 & \text{if } \|\vec{q}\|^6 < 2 \\ 0 & \text{otherwise} \end{cases} \tag{2.2}$$

and $\vec{q}_n$ the centers of the scatterers on the regular triangular lattice.

This system can be considered as a model for electro-conductivity in which the moving particle represents an electron and the scatterer represents the ion of the metal. In the present context it is usually used as a model for color conductivity, where the moving particle has a color charge rather than an electrical charge[5], so that (electrical) interactions between particles, when more than one is present, are avoided. We fix the units in such a way that the mass of the particle is equal to 1, its charge is also equal to 1. The scatterers have a radius of $2^{1/6}$, a distance of 2.5 and the time the particle needs to cover a distance 1 in free space, *i.e.* when not interacting with a scatterer, is $\sqrt{2}$. The last condition just means that the constant energy (kinetic or total) of the particle is fixed to 1. From a mathematical point of view the scatterers are needed to introduce a strong chaos in the system. In general no analytic results are known for this system with respect to its ergodic or chaotic properties. The closest system for which ergodicity and the existence and uniqueness of a limiting distribution (SRB) for the Liouville measure has been proved is the case in which the WCA scatterers are substituted by hard scatterers and the space dimension is 2 (see [13]).

The number of degrees of freedom of the system is three. This means that we have two zero Lyapunov exponents and only 4 non trivial Lyapunov exponents: $\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4$, of which λ_1 and λ_2 are positive, λ_3 and λ_4 negative, if $\vec{E}$ is not too large[12],[13]. If we introduce the pairing error by:

$$p_e = \lambda_1 - \lambda_2 - \lambda_3 + \lambda_4 \tag{2.3}$$

we have for a system for which CPR holds that $p_e = 0$. This implies that we can use p_e as a measure of the discrepancy of the Lyapunov exponents from pairing.

Strictly speaking Lyapunov exponents are defined only in the limit when the time length of a trajectory goes to infinity. Moreover they are only defined almost everywhere with respect to some ergodic measure[14]. In what follows we will use the term local Lyapunov exponent to refer to a definition of a Lyapunov exponent for a single trajectory for a finite time. The particular definition needed will be clear from the context. We will drop the term "local" when no confusion can arise.

In our calculations for the one particle Lorentz model, we focussed our attention on three main points:

A) asymptotic pairing;

B) possibility of generalizing the DM scheme;

C) periodic orbits (see section 3);

A. Asymptotic pairing.

To compute the asymptotic Lyapunov exponents, we calculated the local Lyapunov exponents for as long a time as possible, typically for about 50,000 time units. With our units the time unit equalled the distance unit. We use the standard algorithm[15] consisting of evolving a basic set of unit vectors in the tangent space with the tangent flow and orthonormalizing them from time to time (see [14] for a theoretical justification of this algorithm). It is very hard to give a reliable error estimate on this kind of computation. In fact there are two main sources of error:

1) the intrinsic instability of the dynamical system due to the presence of two positive Lyapunov exponents (quite clear from the simulation) prevents us from following a trajectory of the real system for a long time. In fact even using a very accurate integration method (we used an adaptive step size 4^{th} order Runge-Kutta (RK) integrator with an error control of 10^{-11} at each time step) any truncation error will be exponentially increased. The typical argument to solve this problem is to consider the truncation error as a random perturbation and use the "shadowing lemma" to argue that there must be a trajectory of the real system near by the simulated one[16]. This has, in our opinion, no real mathemathical basis. So we will proceed assuming that the Lyapunov exponents of systems like (2.1) behave continuously with respect to small perturbation-like truncation errors, even if we cannot prove this. We refer to [17] for further discussion.

2) the errors introduced by the numerical round-off in the evaluation of the tangent flow, in orthonormalizing the evolved basis of tangent vectors and the impossibility to do the

infinite time limit on a computer. To deal with this we proceeded in two different ways. The first one was the typical one (see e.g.[18]) and consisted in considering as error the variance of the computed exponent on the last part of the trajectory. The other way was to run more than one simulation, starting from different randomly chosen initial points. We got essentially the same results from both these methods.

To have a clearer idea of the asymptotic values of the Lyapunov exponents, we monitor the 6 local Lyapunov exponents as a function of time for a single trajectory. Using the algorithm of [15], we then have to follow these 6 local Lyapunov exponents. In all cases, we observe that after a short transient time two of them decrease to 0 quite regularly; these two are related to the conservation of energy and the direction of motion. It is natural to consider the remaining four Lyapunov exponents as the non trivial and possibly pairing ones and use the first two (which we will call the zero local Lyapunov exponents) as a check on the precision reached in approaching the infinite time limit. In fact, only when these two zero Lyapunov exponents, λ_0 and λ_{00}, have become approximately equal to zero, can CPR-like behavior be expected to hold for the other four asymptotic-like Lyapunov exponents. We ran simulations both with IK and IE thermostats. Clearly we expect the pairing error for the system with the IK thermostat to go to zero and this can be used as a further check of the precision of the algorithm. The results are reported in Fig. 1.

We see that the three lines in Fig. 1(a) for the IK system approach zero regularly. They can easily be described by a C/t behavior with $C = 1.5$ for the pairing error, $C = 6.0$ for the largest zero exponent λ_0 and $C = 0$ for the smallest exponent λ_{00}. Moreover, pairing is very well satisfied, the pairing error being always smaller than the largest zero exponent λ_0. All this is clearly in good agreement with [1] and reflects the fact that, if one had used a proper Poincaré section on the energy surface and the standard definition of Lyapunov exponents (see [14]), one would have found an identically vanishing pairing error. In this respect, it is interesting to observe that the values and the fluctuations in time of the pairing error are always much smaller than the fluctuations of the largest zero Lyapunov exponent λ_0 (see Fig. 1(c)), again indicating a strong cancellation between the exponents.

In the IE case (Fig. 1b and 1d) we observe again a C/t behavior for the two zero Lyapunov exponents, with $C = 6.0$ and $C = 0$ respectively. However, the pairing error does not show any clear behavior and strongly fluctuates, even after a very long time. Nevertheless, it must be recognized that its value is very small and its fluctuation is of the same order of magnitude as its value. We think that it is very hard to decide on the basis of these data if such a small value is a numerical artifact or a real effect, but we think that the fact that the fluctuations of the pairing error are of the same order of magnitude as those of the maximum Lyapunov exponent, suggest that, even if pairing is obtained, it could not be SCPR in the strong sense of [1].

The results after 50,000 unit of time, with the errors computed from the variance of the last 5,000 time units, are reported in the following table that summarizes the above discussions.

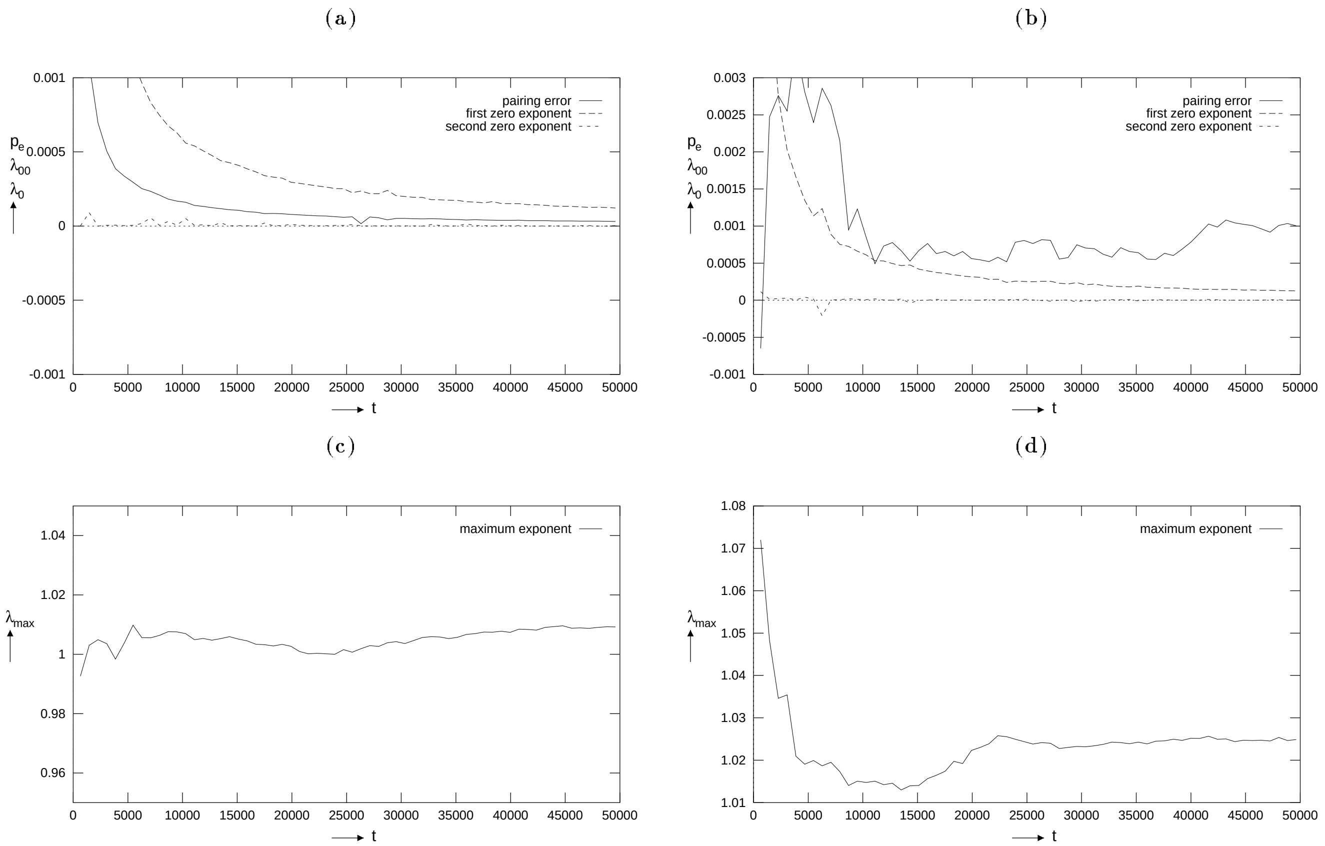

Fig. 1: Behavior, as functions of time, of (a) pairing error, λ_0 and λ_{00} as a function of time for IK Lorentz system (b) same for IE Lorentz system (c) maximum exponent λ_{max} for IK Lorentz system (d) same for IE Lorentz system

	p_e	λ_0	λ_{00}	λ_{max}
IE	$9 \cdot 10^{-4} \pm 3 \cdot 10^{-4}$	$1 \cdot 10^{-4} \pm 2 \cdot 10^{-5}$	$1 \cdot 10^{-6} \pm 9 \cdot 10^{-6}$	$1.0090 \pm 2 \cdot 10^{-4}$
IK	$4 \cdot 10^{-5} \pm 1 \cdot 10^{-5}$	$1 \cdot 10^{-4} \pm 1 \cdot 10^{-5}$	$2 \cdot 10^{-6} \pm 3 \cdot 10^{-6}$	$1.0248 \pm 4 \cdot 10^{-4}$

Table 1: Values for pairing error (p_e) zero Lyapunov exponents (λ_0 and λ_{00}) and maximum Lyapunov exponent (λ_{max}) for IK and IE systems after 50,000 time units

To double check these results we also ran a simulation with 10 different initial conditions, both for the IK and the IE system. The results are given in Fig. 2(a),(b) where we show figures of the behavior of the pairing error p_e for a simulation with ten initial points, plotting the mean value of p_e over the ten points, as well as the maximum and the minimum values observed. We also present the behavior of the maximum Lyapunov exponent in Fig. 2(c),(d) to compare the error of the pairing error with that of the maximum exponent. These results confirm the previous discussion and the errors evaluated with this method are of the same order as those previously reported. Namely: for the IK systems the difference between the maximum and minimum values of the pairing errors is much smaller than those for the maximum Lyapunov exponent, while this is not the case for the IE system. It is interesting to note that after a long time the pairing errors for all the 10 points of the IE simulations are positive. Although not conclusive we do think that this can be considered as strong evidence of non pairing.

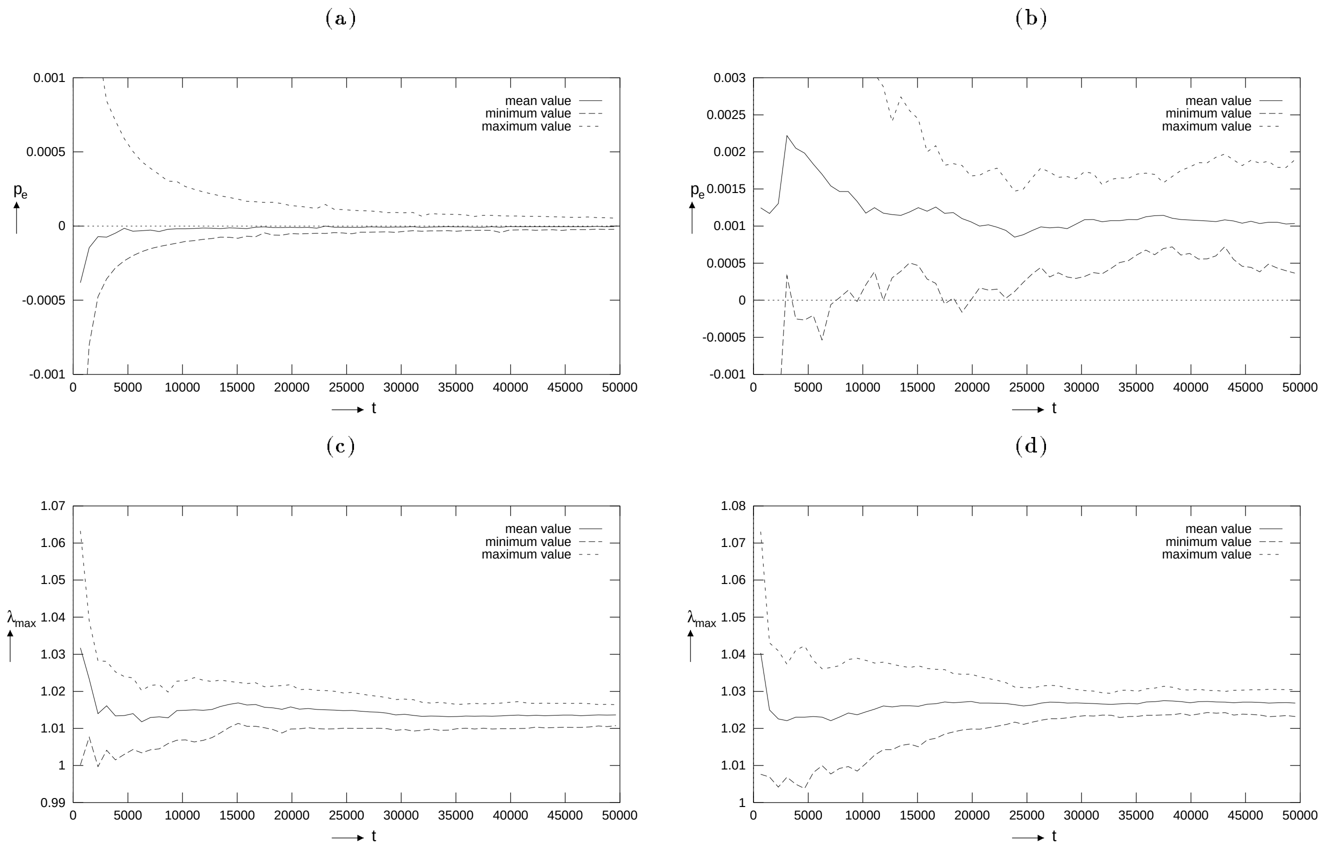

Fig. 2: Behavior of the (a) mean, maximum and minimum values of the pairing error for 10 initial conditions as a function of time for IK system (b) same for IE system (c) mean, maximum and minimum values of the maximum Lyapunov exponent for 10 initial conditions as a function of time for IK system (d) same for IE system

B. Generalizing the DM scheme.

In [1] Dettmann and Morriss consider the flow φ_t on R^{2d} generated by the Hamiltonian IK system (1.1)-(1.2).

The main point in the proof of strong pairing is to split off the two zero Lyapunov exponent associated with the energy conservation and flow direction from the other exponents and then consider the pairing of the other Lyapunov exponents in an appropriate subspace of the full phase space. To eliminate the exponent associated with the energy it is enough to restrict the flow to the energy surface. To get rid of the other exponent we can use a Poincaré section like procedure (see Appendix A2, and figure therein, for a more detailed discussion). This means that given a trajectory, its initial point $\mathbf{x}(0) = (\vec{p}(0), \vec{q}(0))$, a later point $\mathbf{x}(t) = (\vec{p}(t), \vec{q}(t))$ and two corresponding planes $V_{\mathbf{x}(0)}$ and $V_{\mathbf{x}(t)}$ (see Fig. 10), one passing through $\mathbf{x}(0)$ and the other through $\mathbf{x}(t)$, both transversal (i.e. not tangent) to the trajectory, we can consider the map Φ_t induced by the flow φ_t that associates to a point $\mathbf{r}$ on $V_{\mathbf{x}(0)}$ the point $\Phi_t(\mathbf{r})$ on $V_{\mathbf{x}(t)}$ which is the first intersection between the trajectory starting at $\mathbf{r}$ and the plane $V_{\mathbf{x}(t)}$. If we properly choose a plane $V_{\mathbf{x}(t)}$ for any t, the above procedure defines a new flow Φ_t whose Lyapunov spectrum is identical to the one of φ_t but does not contain the zero exponents associated with the flow direction. This is the scheme followed in [1] where it is shown that if one chooses as $V_{\mathbf{x}(t)}$ the plane orthogonal to the vector $J\mathbf{e}_0(t)$ with $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ the usual symplectic matrix and $\mathbf{e}_0(t) = (\vec{p}(t), 0)$ (we will call this choice of V_t the DM subspace), then the eigenvalues of the matrix $L_t^{tr} L_t$ are paired, where the tangent flow $L_t = D\Phi_t$ is the differential of Φ_t (see eq.(A2.2)). From this, the pairing of the Lyapunov exponents for φ_t follows immediately. Observe that $J\mathbf{e}_0$ is a vector field defined on the energy surface with no reference to the particular trajectory. We will call any vector field $\mathbf{g}$, like $J\mathbf{e}_0$ above, such that the eigenvalues of $L_t^{tr} L_t$, given by the above construction, are paired an α-symplectic field. Observe that L_t satisfies an equation of the form:

$$\dot{L}_t = T(\mathbf{x}(t)) L_t \tag{2.4}$$

where $T(\mathbf{x})$ is called the infinitesimal generator of the tangent flow L_t. In [1] it is shown that the matrix $L_t^{tr} L_t$ has paired eigenvalue if $T(\mathbf{x})$ satisfies $JT(\mathbf{x}) + T(\mathbf{x})^{tr} J = -\alpha(\mathbf{x}) J$ for a suitable $\alpha(\mathbf{x})$. If this last condition is satisfied we call L_t and the dynamics that generate L_t α-symplectic and $T(\mathbf{x})$ infinitesimally α-symplectic.

An interesting property of the Lorentz model (with not too high scatterer densities, as considered here) is that the particle spends a significant part of its time in regions where no potential is present, i.e. between two successive interactions with the scatterers. In these regions the IE system is identical to an IK system. It is thus evident that if we consider a trajectory for a time small enough that the particle never interacts with a scatterer, we will find that the local exponents in the DM subspace are paired. Here by local exponents we mean those computed as the eigenvalues of $\frac{1}{2t} \log L_t^{tr} L_t$, where L_t is the differential of the flow (see [14]). A natural question is now that if one considers a trajectory which starts in free space, goes through a collision and then arrives again in free space, can one find again pairing, using the DM subspace? This question is interesting because if there is a α-symplectic field for the IE system, this must give pairing for short (never colliding) trajectories as well as for long trajectories. If no pairing occurs in the DM subspace for long trajectories with collisions, this implies that, even if there is a α-symplectic field for the IE system, there must be either another tranversal symplectic field for the IK system, (at least for the portion of phase space outside the scatterer potentials, *i.e.* in free space) or, alternatively, no DM subspace within which pairing exists for the IE system.

It is not difficult to investigate this question numerically if we consider only a one collision trajectory and we avoid too singular collisions. For, in that case we have only to follow the trajectory for a short time and the diagonalization of the differential of the flow L can be done with very accurately so that we can achieve a precision on the local exponents of 10^{-12} The result is that for the IE system after one collision there is no more pairing in the DM subspace. The interesting point is that the pairing error is of the same order of magnitude as, *i.e.* consistent with, the one observed asymptotically in the long time simulations of Fig. 1, discussed sub A. We were able to go through more than one collision but not through many, because the matrix elements of the tangent flow grow exponentially. Nevertheless for around

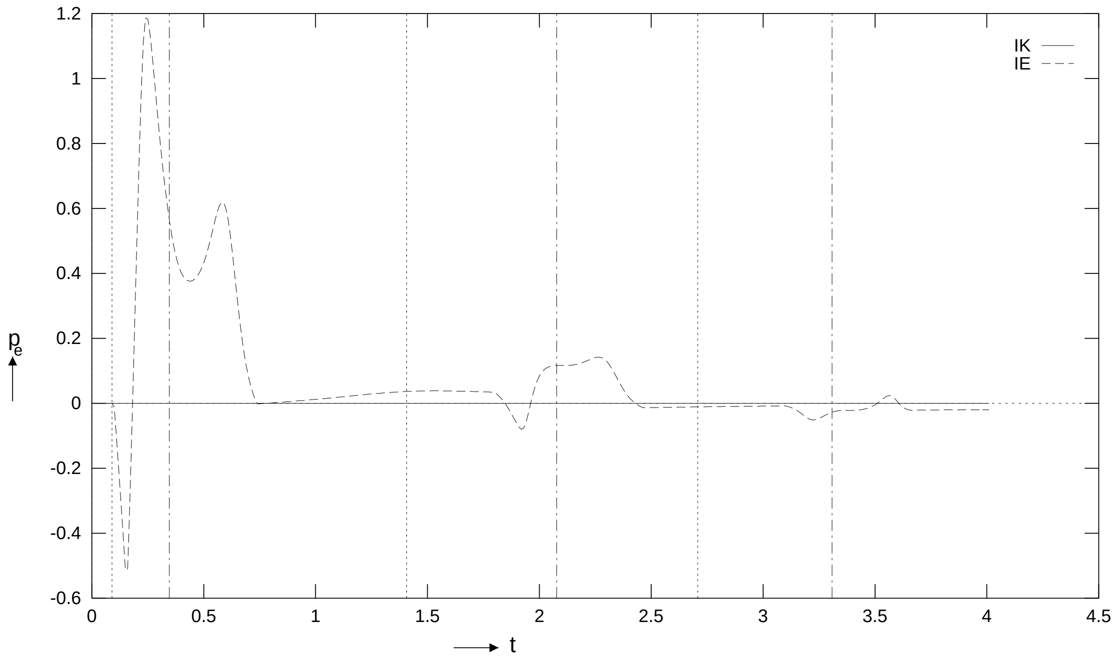

Fig. 3: Behavior of the pairing error as function of time during a few interaction with the scatteres for the IK (identically 0) and IE system. The time which the particle enters and leaves the potential of a scatterer are indicated by vertical lines of two different dashing (the particle start outside all the potentials).

three collisions, one sees that the pairing error in the DM space is always violated by more or less the same amount, most during collisions and decreasing during free flight (cf. Fig. 3).

The question of the existence of a possibly different transversal symplectic field for the IE Lorentz system is nonetheless still open but this is clearly a question that is not easily investigated numerically. We chose to look at a similar but in principle simpler alternative: given a point $\mathbf{x}(0) = (\vec{p}(0), \vec{q}(0))$ and a tangent vector $\mathbf{w}(0)$, at $\mathbf{x}(0)$ is it possible to find a vector $\mathbf{w}(t)$ tangent at $\mathbf{x}(t)$ such that the linearized flow from the orthogonal to $\mathbf{w}(0)$ to the orthogonal to $\mathbf{w}(t)$ has paired local Lyapunov exponents? This means computing the linearized flow for a time t starting from $\mathbf{x}(0)$ and then looking for a solution of the equation $p_e(\mathbf{w}(t)) = 0$ (where we consider the pairing error as a function of $\mathbf{w}(t)$). Observe that this equation depends on four variables, while a unique condition is imposed so that if a solution exists it will generically not be unique. Note that the existence of $\mathbf{w}(0)$ and $\mathbf{w}(t)$ for any initial point $\mathbf{x}(0)$ and t does not imply that these vectors generate a vector field on the energy surface (like is the case in the DM proof, see Appendix A2). However, this would be enough to prove SCPR, if one also had that $\mathbf{w}(t)$ does not become orthogonal to $\dot{\mathbf{x}}(t)$

The problem with this computation is that we can handle only short times t for the same reasons as given above, namely that the matrix elements of the tangent flow grow exponentially with the maximum Lyapunov exponent while we want to compute a function of them, *i.e.* the minimum eigenvalue, which decreases exponentially with the minimum Lyapunov exponent.

In our simulations we followed the trajectory for a time 10 (i.e., for 5 to 7 collisions) computing $\mathbf{w}(t)$ for $t = n\delta t$ with $\delta t = 0.1$ and $n = 1, 2, 3, 4, ...$ The initial point was chosen outside all the scattering potentials in such a way that the choice $\mathbf{w}(0) = J\mathbf{e}_0(0)$ was a natural one. To obtain $\mathbf{w}(t)$, we started with JDH_0 (see (1.5),(1.6) and (A2.2)) looking for a solution with a steepest-descent method, till the pairing error changed sign and then using bisection. Observe that in this setting the algorithm applied to the IK system would be completely trivial. We also tried to find other solutions for example using as an initial attempt for $\mathbf{w}(t)$ at t the last computed $\mathbf{w}(t-\delta t)$ at $t-\delta t$. We note that this is also a possibly interesting procedure for the IK case because the result need not be $J\mathbf{e}_0(t)$, as would be the case for [1].

In fact, in all cases we were always able to find the vector $\mathbf{w}(t)$. That it was also possible for the IK system to find a $\mathbf{w}(t)$ different from $J\mathbf{e}_0(t)$ which satisfies the pairing rule (at least for a short time t) could lead to a different scheme to prove CPR for the IK system in a possibly more general fashion than in [1]. Unfortunately we were unable to prove this and our numerical simulations were too short to give real insight into the above question.

3. Periodic orbits

To obtain a more or less definitive result on the possibility of having pairing for all time and all initial conditions, we decided to check the pairing of the Lyapunov exponents on periodic orbits of the single particle periodic Lorentz gas, considering that periodic orbits solve the problem of obtaining truly asymptotic Lyapunov exponents, since the asymptotic Lyapunov exponents on a periodic orbit are just the logarithms of the modulus of the eigenvalues of the differential of the flow after a period, divided by the period. However, errors are introduced in finding periodic orbits numerically. Having a periodic orbit or an orbit we know is near enough to a periodic orbit, will permit us to obtain a very good estimate of the error involved in the computation of the asymptotic Lyapunov exponents. In fact, if the period of the orbit is not too long the exponential propagation of errors can be controlled with an accurate integration scheme (we again used a 4^{th} order RK with adaptive step size with error under 10^{-14}). Having to diagonalize a matrix only once, these operations do not increase the error significantly for sufficiently short periodic orbits, because, after a short time, the matrix elements of the differential of the flow are not yet very large. The real problem is to find the best approximate periodic orbits numerically and to estimate their deviations from real periodic orbits.

To this end we ran a long time single particle trajectory and recorded the positions of the particle when it entered in the interaction (WCA) potential of a scatterer (we will register this as a collision). In this way we get a long list $\mathbf{x}_n$ of collision points and, fixing a period T, we look for all m such that $|\mathbf{x}_m - \mathbf{x}_{m+T}| < \epsilon$ for some ϵ (10^{-2} in our experiments). We then search for a periodic orbit near this orbit using the Newton-Ramson method. The algorithm stops when the distance between the initial and the T-th collision point is less than 10^{-12}.

Having a small distance between the initial and the final point of the orbit does not automatically ensure that the orbit is near a periodic one. A good check of this is to see if the application of the Newton-Ramson method gives a quadratic convergence as should theoretically be the case[19]. This means that iterating the method, if the error at the n-th step is ϵ, it should be $C\epsilon^2$ at the $(n+1)$-th step, where C is a constant linked to the first and second derivatives of the flow. Another good check is to see whether in the computed Lyapunov spectrum there are two 0 exponents (which means that the spectrum of the differential of the flow must contain two eigenvalues 1 with sufficient precision. Both these conditions were always fulfilled in our computations: every time a periodic orbit was found, the algorithm converged quadratically and there were always two eigenvalues with logarithms of the order of 10^{-12}. We think that the error on the evaluated exponents can be conservatively estimated as less than 10^{-9}.

We found typically about 200 periodic orbits for periods ranging from 2 to 8. For all these periods it was possible to find periodic orbits whose exponents were not paired by an amount significativelly larger than the expected error. We report in the following table a number of relevant quantities we have observed for each period for the two periodic orbits with the largest pairing errors.

	pairing level	pairing value	relative pairing error
Period 2	-0.038903	0.081320	-2.090341
	0.005453	-0.528786	-0.010312
Period 3	-0.388106	0.074560	-0.192114
	0.061834	-0.313116	-0.197480
Period 4	-0.339775	0.157961	-0.464897
	0.144549	-0.256445	-0.563666
Period 5	-0.271768	0.093026	-0.342300
	0.084853	-0.259349	-0.327179
Period 6	-0.397877	0.119123	-0.299397
	0.097328	-0.352683	-0.275963
Period 7	-0.338662	0.022185	-0.065507
	0.020747	-0.438584	-0.047305
Period 8	-0.467454	0.030299	-0.064817
	0.020875	-0.525150	-0.039751

Table 2: Pairing value $-\langle\alpha_{IE}\rangle_t$, pairing error (eq.(2.3)) and relative pairing error (ratio of the pairing error to the pairing level, i.e. of columns 2 and 1) for each period of the 2 periodic orbits with the largest pairing errors.

These results provide a numerical proof that SCPR for the one particle IE Lorentz model cannot be true, so that no proof like that of [1] is possible for this system. Nevertheless we note that this does not rule out the possibility of asymptotic pairing with respect to an ergodic measure. In fact, periodic orbits are a set of measure zero so that even if no periodic orbit has paired Lyapunov exponents, this does not imply that the asymptotic Lyapunov exponents for $T \to \infty$ are not paired.

We note that the behavior of periodic orbits can also lead to a better understanding of the general behavior of the system. First, there is apparently a large difference between the behavior of orbits with even and odd periods (even or odd refers here to the number of collisions on an orbit). In fact, while almost all period 3 orbits have a quite large pairing error, those of even period have predominantly a zero pairing error (i.e. smaller than the precision of the algorithm and often actually evaluated as zero). To show this effect we made histograms of the probability $Pr(p_e)$ of finding an orbit with a pairing error p_e, *i.e.* the number of orbits found with that pairing error divided by the total number of orbits found. The results are shown in Fig. 4.

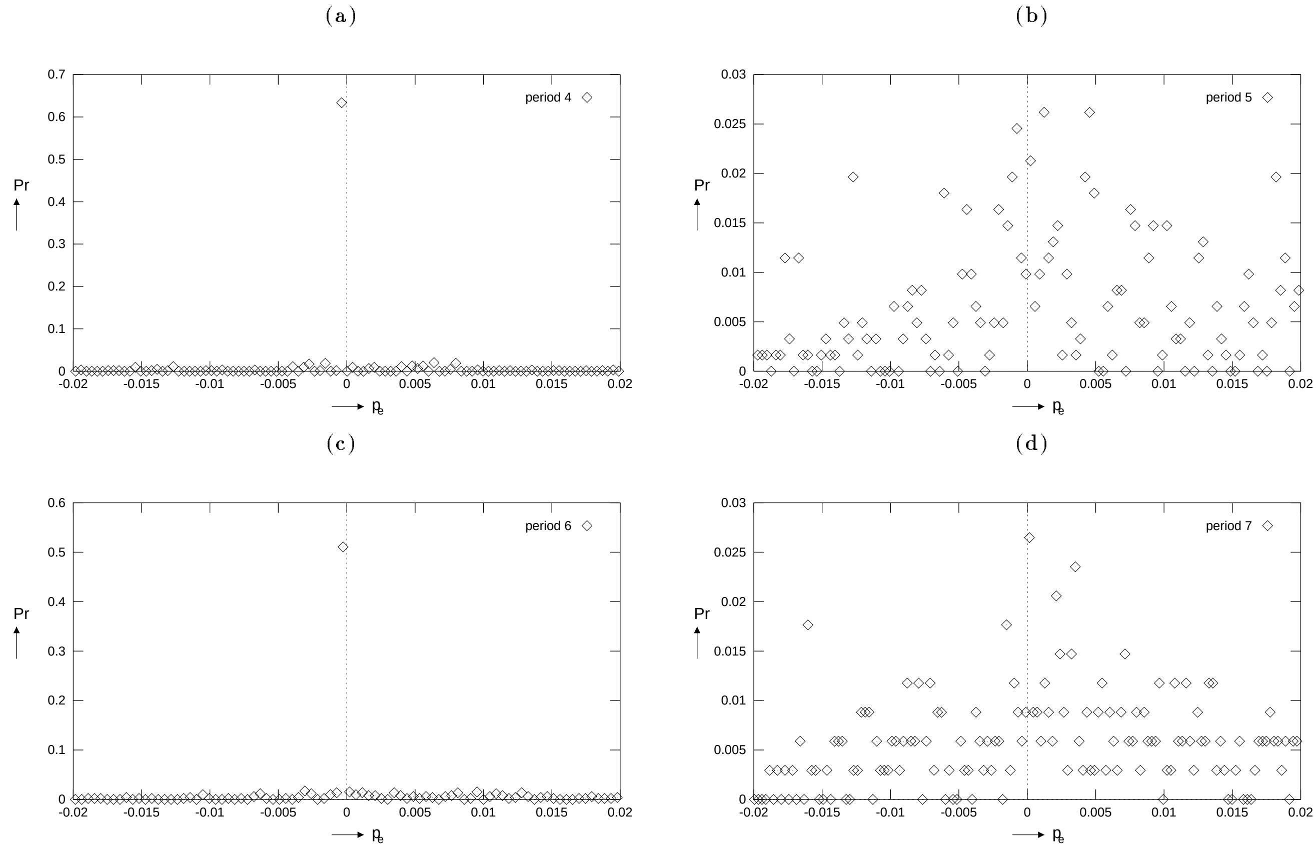

Fig. 4: Distribution of the pairing error for orbits of period (a) 4 (b) 5 (c) 6 (d) 7. In fig.4(a) the single point at about 0.65 means that about 65% of the periodic orbits with period 4 have approximately zero pairing error, while in Fig. 4(b) only about 1% of the periodic orbits have a pairing error near zero. The apparently layered structure of the histograms in Figs 4(b),(d) is due to the relatively small intervals chosen in the histograms.

Secondly, we note that the existence of many even periodic orbits with paired Lyapunov exponents can perhaps be connected with some generalization of the [1] proof of pairing. We hope to come back to this point in a future paper.

4. Many particle systems.

In the previous sections we have seen that that no SCPR holds for a particular Hamiltonian IE system, i.e. the one particle Lorentz model. In particular, the numerical results on periodic orbits seem to establish that even asymptotic pairing is violated. In order to investigate the effect on pairing in the presence of more than one particle, in fact of many particles, we looked at the same model but with more than one particle moving among the scatterers. We considered color diffusion in an external field, putting no interaction potential between the particles in order to be able to make very long and careful simulations, as well as for other reasons that will become clear in what follows. Observe that when a thermostat is added to this system of non-interacting particles, the particles are no more independent, because the thermostat (IK or IE) constraint introduces an indirect interaction between them.

The equation of motions of this system are again (1.1)-(1.2) with $N > 1$ (we will use $N = 2, 3, 8, 16, 32$), $\phi^{ext}(\underline{q}) = \sum_{i=1}^{N}(\vec{E}, \vec{q}_i)$, using the same notation as in sec. 2 (see comment above eq.(2.1)) and $\phi^{int}(\underline{q}) = \sum_{i=1}^{N}\phi^{WCA}(\vec{q}_i)$ with $\phi^{WCA}(\vec{q})$ given by eqs.(2.1)(2.2). The units are fixed as in sec. 2 (see comments after eq.(2.2)).

In this setting it is possible to consider also a different kind of thermostat, which we will call an isopeculiar kinetic (IPK) thermostat, which is, in general, more physical, but has no meaning for a single particle. It consists, in constraining only the peculiar (i.e., thermal) kinetic energy, i.e the kinetic energy with respect to the center of mass of the moving particles. The equations of motion one then obtains are $(i = 1, ..., N)$:

$$\begin{cases} \dot{\vec{q}}_i = \dfrac{\vec{p}_i}{m} \\ \dot{\vec{p}}_i = \vec{f}^{WCA}(\vec{q}_i) + \vec{E} - \alpha_{IPK}(\underline{p}, \underline{q})\tilde{\vec{p}}_i \end{cases} \tag{4.1}$$

where $\vec{f}^{WCA}(\vec{q}) = \partial\phi^{WCA}(\vec{q})/partial\vec{q}$ and

$$\tilde{\vec{p}}_i = \vec{p}_i - \frac{1}{N}\sum_{j=1}^{N}\vec{p}_j$$

is the peculiar momentum and

$$\alpha_{IPK}(\underline{p}, \underline{q}) = \frac{\sum_i(\tilde{\vec{p}}_i, \vec{f}^{WCA}(\vec{q}_i))}{\sum_i \tilde{\vec{p}}_i^{\,2}} \tag{4.2}$$

The main reason to look at a many particle system is the idea that the CPR could be valid only in the limit that the number of particles goes to infinity, which would suffice for statistical mechanics. There are two kinds of evidences for this point. The first is based on many numerical simulations, in which the Lyapunov spectrum of a many particle system is computed and a good agreement with the pairing rule is obtained, see [5][7][6]. However, considering the small deviations observed in sec. 2 and the periodic orbit results, it seems doubtful that those simulations can really establish pairing definitively.

A second reason arises from an analytic argument that was first presented in [7]. We give here a more rigorous and extended presentation of that argument.

Suppose we have an IE system given by a Hamiltonian of the form eq.(1.1), equations of motion eq.(1.2) with thermostat eq.(1.4). In Section 2, sub B, following [1], conditions for pairing of an IK system to hold were tied to finding a proper subspace. As was pointed out before the argument for choosing the proper subspace was related to the need of taking out of the spectrum the two zero eigenvalues that are always present, but pair to a different constant ($\neq 0$) than the other Lyapunov exponents. However, since we have been unable to find the proper CPR subspace for the IE system, we were forced (as in the previous section) to proceed in the full phase space, replacing, in a way, the proper subspace by the condition that the zero Lyapunov exponents $\lambda_0 \approx \lambda_{00}$ must be ≈ 0 in the full phase space calculations for CPR to hold.

We can now consider the tangent flow associated with these equations but, instead of looking at it in an appropriately chosen transversal subspace, like we did in sec. 2, we look, in the spirit of the previous section, at the tangent flow in the full phase space. Let us call again $\varphi_t(\mathbf{x})$ the flow generated by eq.(1.2) and $L_t = D\varphi_t$ the tangent flow. Then L_t satisfies an equation identical to eq.(2.4), with $\mathbf{x} = (\underline{p}, \underline{q})$:

$$\dot{L}_t = T(\mathbf{x}(t))L_t \tag{4.3}$$

(we use here the same convenient notation in full phase space as we did in the DM subspace of sec.2 for slightly different objects, because we think that no confusion can arise). The matrix $T(\mathbf{x})$, the infinitesimal generator of the tangent flow, has the simple form:

$$T(\mathbf{x}) = T_H(\mathbf{x}) - \alpha_{IE}(\mathbf{x})I_{\underline{p}} - \underline{p} \otimes \underline{\nabla}\alpha_{IE}(\mathbf{x}) \tag{4.4}$$

where T_H is the infinitesimal generator of the tangent flow for the Hamiltonian system, i.e. $T_H = J\underline{\partial}^2 H$ with J the usual symplectic matrix and $\underline{\partial}^2 H$ the matrix of the second derivatives of H with respect to all momenta and positions. Moreover $I_{\underline{p}} = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}$, i.e. the identity on the $\underline{p}$ subspace and $\otimes$ represents the tensor (or dyadic) product. It is easy to see that if we neglect the term $\underline{p} \otimes \underline{\nabla}\alpha_{IE}(\mathbf{x})$ the matrix $\check{T}(\mathbf{x}) = T_H(\mathbf{x}) - \alpha_{IE}(\mathbf{x})I_{\underline{p}}$ satisfies the relation:

$$J\check{T}(\mathbf{x}) + \check{T}^{tr}(\mathbf{x})J = -\alpha_{IE}(\mathbf{x})J \tag{4.5}$$

where $\check{T}^{tr}(\mathbf{x})$ is the transpose of $\check{T}(\mathbf{x})$. This follows from the fact that for a Hamiltonian system $JT_H(\mathbf{x}) + T_H(\mathbf{x})^{tr}J = 0$ and $JI_{\underline{p}} + I_{\underline{p}}^{tr}J = J$. This, in turn, implies that if we consider the characteristic exponents[14] associated with the matrix $\check{T}(\mathbf{x})$, which we will call the mutilated spectrum of the system, they will be paired. This follows directly, for example, from the last part of [1], or from [7] and the pairing level will be exactly equal to $-<\alpha_{IE}>_t$. Moreover for these exponents a SCPR holds. Note that the mutilated spectrum does not necessarily have two zero exponents. This creates a first difference between the (true) Lyapunov exponents spectrum and the (mutilated) characteristic exponents spectrum, but we expect that the two zero Lyapunov exponents associated with $T(\mathbf{x})$ will be converted into a couple of paired mutilated characteristic exponents associated with $\tilde{T}(\mathbf{x})$, one of which is numerically found to be zero, while the other one equals twice the pairing level $-<\alpha_{IE}>_t$

(see Fig. 7 and discussion below it). The critical question is whether the term $\underline{p} \otimes \underline{\nabla}\alpha(\mathbf{x})$ can be neglected. Observe that

$$
\begin{aligned}
\frac{\partial \alpha_{IE}(\mathbf{x})}{\partial \vec{p}_i} &= \frac{f_i^{ext}(\underline{q})}{\sum_j \vec{p}_j^{\,2}} + \alpha_{IE}(\mathbf{x}) \frac{\vec{p}_i}{\sum_j \vec{p}_i^{\,2}} \\
\frac{\partial \alpha_{IE}(\mathbf{x})}{\partial \vec{q}_i} &= 0
\end{aligned}
\tag{4.6}
$$

If we go to the thermodynamic limit, keeping the energy per particle fixed, we will have that, in the mean $\sum_j \vec{p}_j^{\,2} \simeq N||\vec{p}_i||$, so that we can say that $\underline{\nabla}\alpha_{IE}$ is of the order of $1/N$. Although this makes the above procedure more reasonable, it is mathematically not justified. A similar argument holds for IPK thermostatted systems. In fact we have in that case:

$$
T^{IPK}(\mathbf{x}) = T_H(\mathbf{x}) - \alpha_{IPK}(\mathbf{x})\tilde{I}_{\tilde{p}} - \underline{\tilde{p}} \otimes \underline{\nabla}\alpha_{IPK}(\mathbf{x}) \tag{4.7}
$$

where $\tilde{I}_{\underline{\tilde{p}}} = I_{\underline{p}} + O(1/N)$ and $\underline{\nabla}\alpha_{IPK}(\mathbf{x})$ is given by slightly more complicated expressions than eq.(4.6), but can still be considered as being $O(1/N)$.

The $1/N$-argument has three major problems:

a) It is mathematically speaking not always true that $\frac{\partial \alpha_{IE}}{\partial \vec{p}_i} = O(1/N)$. For, in the IE case it can happen that $\sum_j \vec{p}_i^{\,2}$ is very small or even zero, if all the energy of the system is potential energy, so that the system has no kinetic energy. This implies then that the first term in eq.(4.6) can be very large. Of course, it will nevertheless be true that for most parts of phase space $\sum_j \vec{p}_j^{\,2}$ is $O(N)$ and the volume of the region where it is small will go to zero as the number of particle goes to infinity. This effect is not present in the IPK system, because in the denominator of α_{IPK} the constrained quantity itself then appears.

2) If we consider the two equations

$$
\dot{L}_t = T_t L_t \qquad\qquad \dot{\check{L}}_t = \check{T}_t \check{L}_t
$$

where $\check{T} = T + O(1/N)$, it is not generically true that $\check{L}_t = L_t + O(1/N)$ uniformly in t. In fact we will typically have that

$$
\check{L}_t = L_t + f(t)O(1/N) \tag{4.8}
$$

for some $f(t)$. The point is then to control the growth of $f(t)$, but this is, generically, very hard.

3) Even assuming that we could prove (4.8), it is easy to give an example of matrices of the form $\check{L}_N = L_N + (1/N)P_N$ in which the spectrum of $\check{L}_N$ is completely different from that of L_N. Let L_N a Jordan block with eigenvalue a. That is $(L_N)_{i,i} = a, (L_N)_{i,i+1} = 1$, while all other matrix elements are zero. Let $(P_N)_{N,1} = 1$ while all other matrix elements

of P_N are zero, i.e.,

$$L_N = \begin{pmatrix} a & 1 & 0 & \cdots & 0 & 0 \\ 0 & a & 1 & \cdots & 0 & 0 \\ 0 & 0 & a & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a & 1 \\ 0 & 0 & 0 & \cdots & 0 & a \end{pmatrix} \qquad P_N = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & \cdots & 0 \end{pmatrix}$$

Using the properties of triangular matrices it is easy to see that the spectrum of L_N consists then only of the point a counted with multiplicity N, while the eigenvalues λ_i of $\check{L}_N$ are given by $\lambda_i = N^{-\frac{1}{N}} u_{i,N}$ where $u_{i,N}$ are the N-th root of the unity, *i.e.* $u_{i,N}^N = 1$. This implies that the spectrum of $\check{L}_N$ converge to the circle in the complex plane of radius 1 with center at a, when N goes to infinity. Moreover, if we replace the perturbation $O(N^{-1})$ by a perturbation $O(f(N)^{-1})$ we need essentially that $\lim_{N\to\infty} \frac{f(N)}{\exp(N)} = \infty$ for the spectrum of $\check{L}_N$ to coincide with that of L_N, i.e., any perturbation of the form N^{-p} for a fixed p will give the same result. This is clearly connected with the existence of many degenerate eigenvalues, but it is not clear that a hypothesis of non degeneracy would be enough to give convergence of the spectrum of $\check{L}_N$ to that of L_N.

Since we were not able to decide analytically the above points, which are well known difficulties if one tries to prove continuity of characteristic exponents with respect to perturbations, we checked the behavior of the Lyapunov exponents as a function of N numerically. We did simulations for $N = 2, 4, 8, 16$ and 32 particles. In this case it became not feasible to run simulations for 10 different initial conditions, because the 16 and 32 particle simulations already needed two weeks of CPU time. So we computed errors by only looking at the fluctuations in the last part of the trajectory (see sect. 2) and we always ran analogous simulations for the IK model to check the precision of the program. Moreover the lengths of the simulations were necessarily shorter than those used for the single particle system. Observe that, for the IE system, because of the absence of interactions among the particles, if we neglect the term containing the derivatives of α, the matrix $\check{T}$ splits into a block matrix consisting on N blocks of dimension 6×6 on the principal diagonal of the matrix. This, assuming ergodicity, implies that the mutilated spectrum for this system consists of only 6 different characteristic exponents, each of which is N times degenerate. This allows a very easy check on the convergence of the spectra of the characteristic exponents associated with $\check{T}$, as N goes to infinity.

Fig. 5 shows the behavior of the pairing error as a function of time, each graph reporting the observed pairing error for the IK, IE, IPK system at a fixed number of particles. To make the comparison more informative we decided to plot the behavior of the ratio Π_e between the pairing error P_e and $- < \alpha >_t$, i.e. the value at which the exponents would pair if pairing were to occur. Observe that in this situation the number of pairs is no more 2, as it was in the one particle system. Therefore, we adopted as a definition of pairing error the variance of the values observed, i.e. calling $m_i = \lambda_i + \lambda_{6N-2-i}$ we set

$$P_e = \frac{1}{N}\sum_i m_i^2 - \left(\frac{1}{N}\sum_i m_i\right)^2 \tag{4.9}$$

.

Observe that the behavior in time of the pairing error for the IE and IPK systems becomes more and more regular and similar to that of the IK system as the number of particles increases. In section 2 we saw that the smooth behavior of the pairing error of the form C/t for the IK system can be deduced from the existence of strong cancellations leading to a proof of SCPR. This suggests that a form of SCPR could hold when the number of particle goes to infinity or, at least, that the local Lyapunov exponents in a proper subspace will pair faster and faster in time.

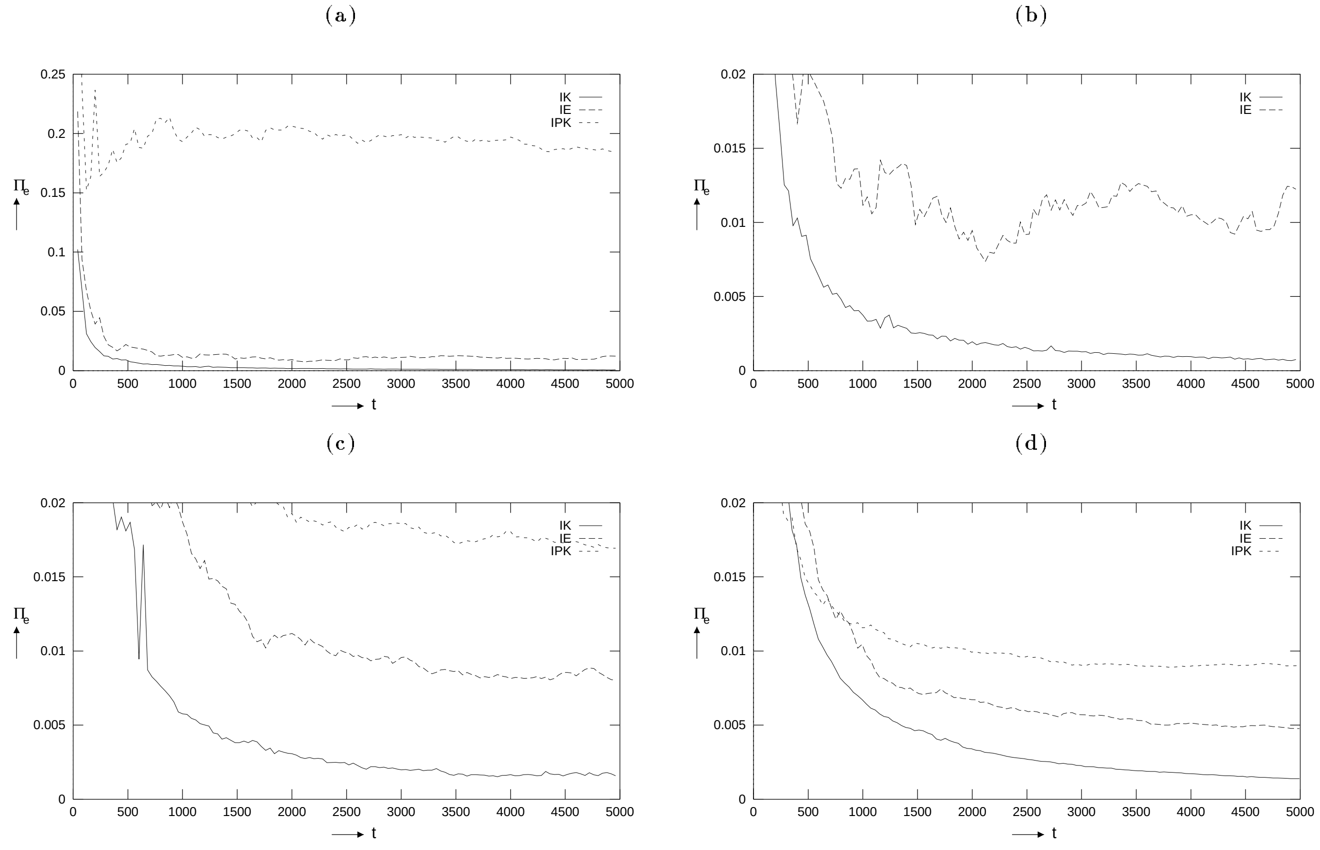

Fig. 5: Behavior of ratio Π_e of the pairing error P_e and $- < \alpha >_t$ as a function of time, for the IK, IE, IPK systems with (a) 2 particles; (b) IK, IE of (a) on a finer scale; (c) 8 particles; (d) 32 particles.

In Fig. 6 we report the values after 5,000 time units for Π_e of the three systems as a function of the number of particles N.

We see that the pairing error for the IK, IE and the IPK systems is a decreasing function of N. Moreover the final value of the last two systems gets closer to the final value obtained for the IK system, where we know that the exponents should be paired. Thus it appears that our simulations are consistent with pairing for the IE system in the thermodynamic limit.

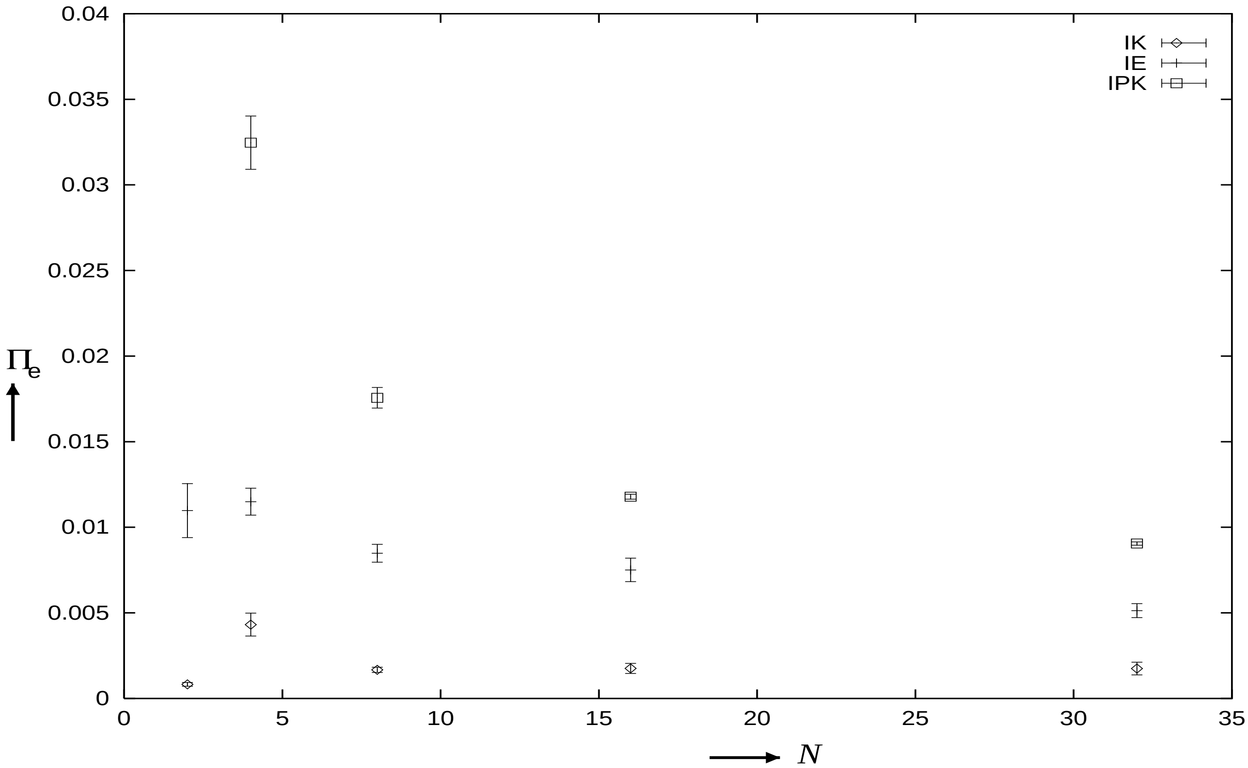

Fig. 6: Ratio Π_e of the pairing error P_e and $- < \alpha >_t$ as a function of the number of particles for the IK, IE, IPK systems. The IK values provide an estimate of the computer program accuracy, since they should vanish.

Finally, as noted before, the characteristic exponents associated with the matrix $\check{T}$ have a particularly simple structure and are quite easy to evaluate. So we checked to what extent the Lyapunov spectrum converges to this simple spectrum. Fig. 7 reports the results for the IE system while Fig. 8 reports those for the IPK system. Note that in these figures only $3N-1$ pairs of exponents are shown, because one pair can be easily deduced, *i.e.* it is a pair of zero exponents for the Lyapunov spectrum, while it is identical to the $(3N-1)$-th for the mutilated spectrum. Moreover, one would expect in general that the IE system and the IK system would become more and more similar as the number of particles goes to infinity. This is indeed seen in Fig. 9. Note that this argument does not apply to the IPK case. In fact this thermostat has a different and more physical nature in that the velocity of the center of mass is not constrained and only the energy with respect to the center of mass is fixed, so that we cannot expect any equivalence between the IE or IK systems and the IPK system.

Both Figs 7 and 8 show a weak similarity of the spectrum associated with the matrix $\check{T}$ and the real Lyapunov spectrum. However, the two spectra do not seem to converge to each other for $N \to \infty$. The spectra of both models could in principle both split for $N \to \infty$ into six straight segments, an indication of which is visible in Fig. 7, at two thirds of the Lyapunov spectrum. Since it is rather unlikely that the spectrum associated with T will become discontinuous when $N \to \infty$, it seems much more likely that the discontinuous spectrum associated with $\check{T}$ will become continuous, if direct interactions between the particles are introduced. It is interesting to note that the two systems appear to pair to the same value and it is almost impossible to see from the figures whether the exponents are exactly paired or not. The observed pairing error of the Lyapunov spectrum is so small that any deviation of pairing

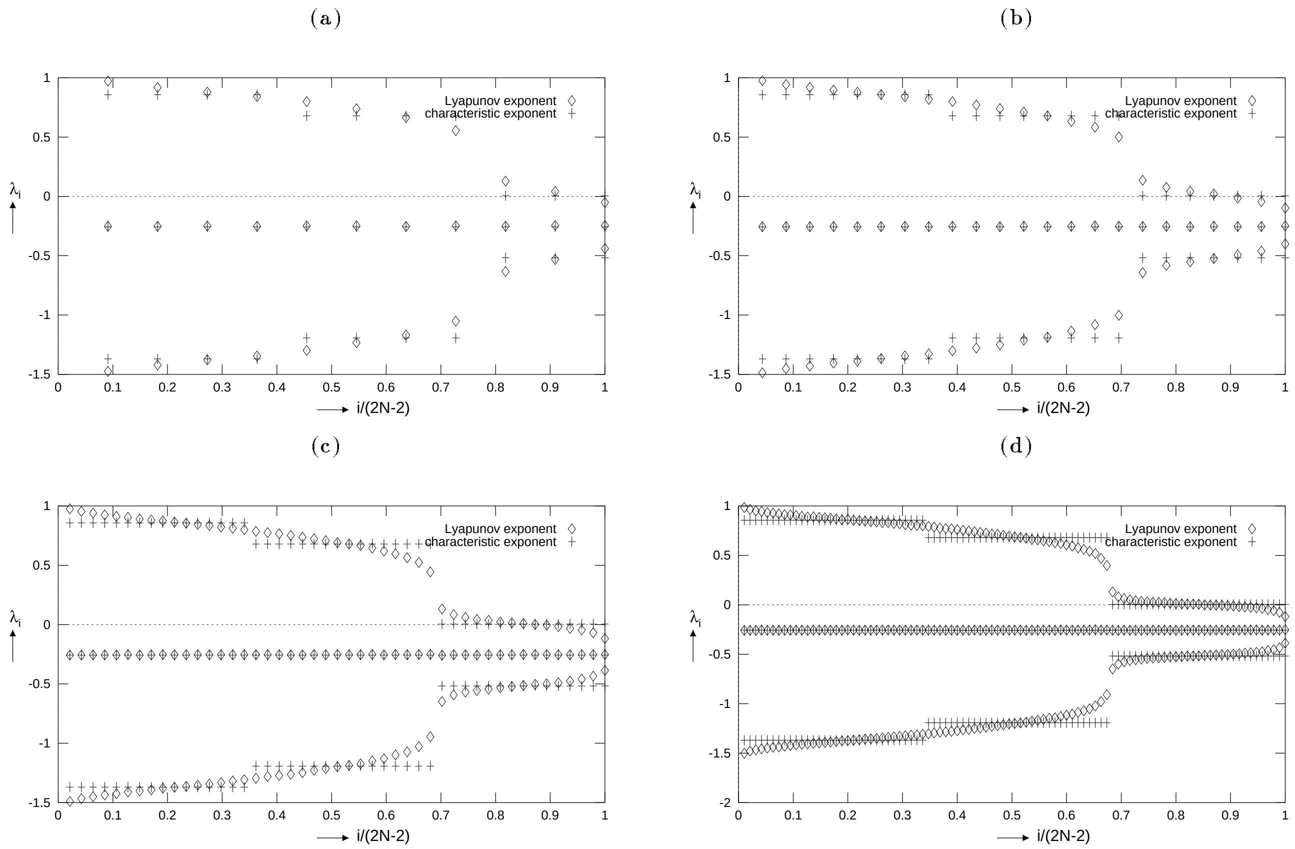

Fig. 7: Comparison of the Lyapunov spectrum λ_i of an IE system with the spectrum of characteristic exponents associated with $\check{T}$ for (a) 4 particles; (b) 8 particles; (c) 16 particles; (d) 32 particles.

could well be due to numerical errors or to too short a simulation time. The same cannot be said of the spectrum themselves.

Finally we discuss Fig. 9. A generalization of the idea of the equivalence of ensembles for large N, discussed formally in a different context by a number of authors[20], makes it quite reasonable to surmise that the IE and IK systems should become equivalent for sufficiently large N. This is quite consistent with our computations. We see that the mean phase space contraction $- < \alpha >_t$ is the same for the two thermostatted system, while the two spectra agree very well for the larger exponents, differing only slightly for the smaller exponents, in the latter parts of the spectra.

5. Discussion

1. One of the main results of this paper is the numerical proof of the non validity of SCPR for a one particle Lorentz gas. This is obtained through a careful evaluation of periodic orbits, keeping meticulously track of the computational errors. In fact, Lyapunov exponents for periodic orbits can be computed with very high accuracy if the periodic orbit is not too long. The existence of periodic orbits that do not satisfy the strong pairing rule shows that SCPR is not valid. We also note that periodic orbits form a set of measure zero. This

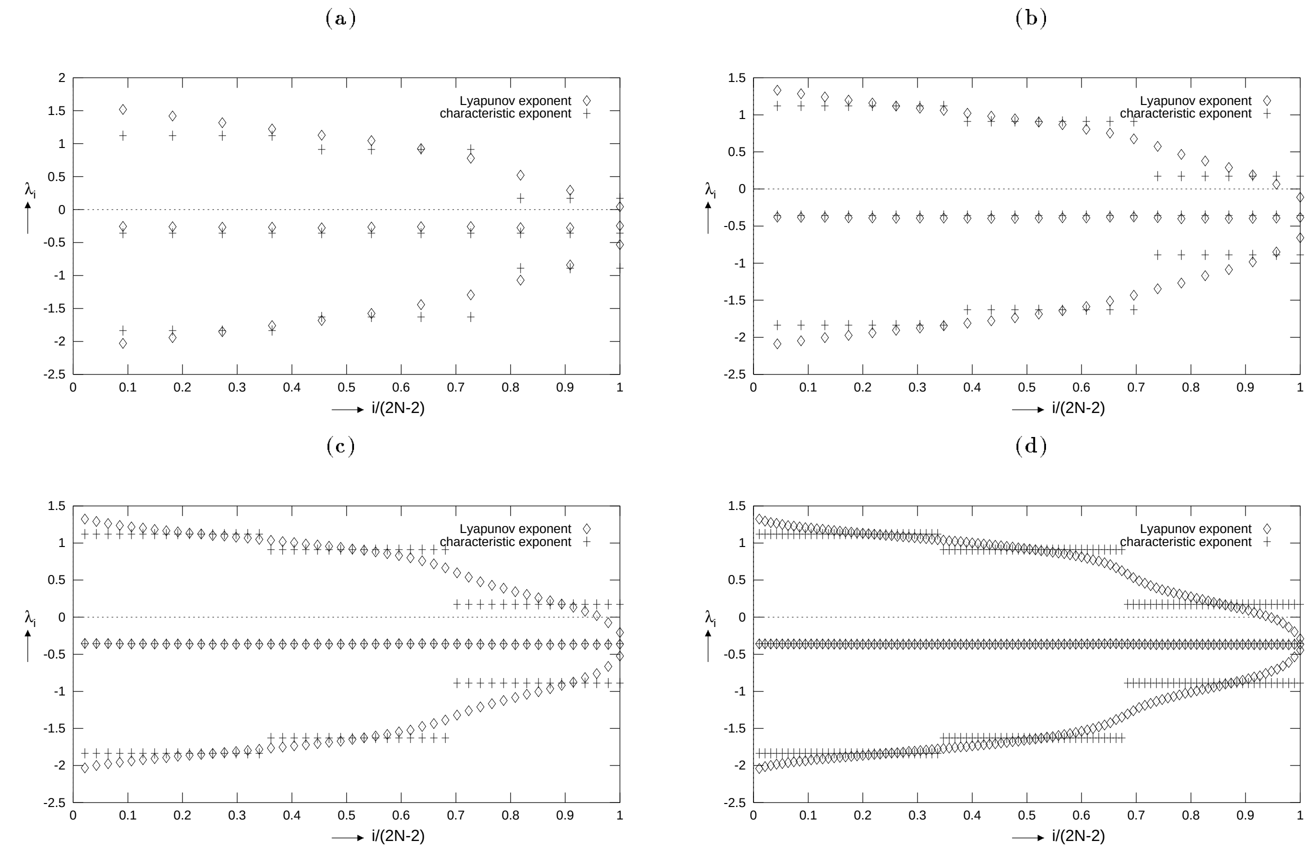

Fig. 8: Comparison of the Lyapunov spectrum λ_i of an IPK system with the spectrum of characteristic exponents associated with $\check{T}$ for (a) 4 particles (b) 8 particles (c) 16 particles (d) 32 particles.

implies that no conclusion as to asymptotic pairing of non-periodic trajectories can be drawn from the above observations. Nevertheless the violation of pairing in periodic orbits is consistent with the results of the very long simulations for non-periodic trajectories of Section 2, used to compute asymptotic Lyapunov exponents. Also these simulations showed deviations from pairing for the IE systems, but the deviations were too small to identify clearly a real effect, because of the numerical errors always associated with this kind of simulations.

2. We have also tried to generalize the DM scheme for proving strong pairing. This lead to a reformulation of the proofs in [1], [2] and [8] by one of us (C.P.). With reference to the discussion and notation of sec. 2 sub B, we call a vector field $\mathbf{g}$ for the flow φ_t defined on the energy surface α-symplectic if the eigenvalues of $L_t^{tr}(\mathbf{x})L_t(\mathbf{x})$ are paired, where L_t is the linearized flow for the trajectory starting at $\mathbf{x}$. Then it was possible to give a necessary and sufficient condition on $\mathbf{g}$ to be α-symplectic directly in terms of the equations of motion . More precisely, calling $V_{\mathbf{x}}$ the plane orthogonal to $\mathbf{g}(\mathbf{x})$ in the point $\mathbf{x}$ and $T(\mathbf{x}) = \frac{d}{dt}L_t(\mathbf{x})\Big|_{t=0}$, this implies that there must exist a function $\alpha(\mathbf{x})$, such that the matrix $M(\mathbf{x}) = JT(\mathbf{x}) + T^{tr}(\mathbf{x})J$ satisfies:

$$(\mathbf{w}, M(\mathbf{x})\mathbf{w}') = \alpha(\mathbf{x})(\mathbf{w}, \mathbf{w}') \tag{5.1}$$

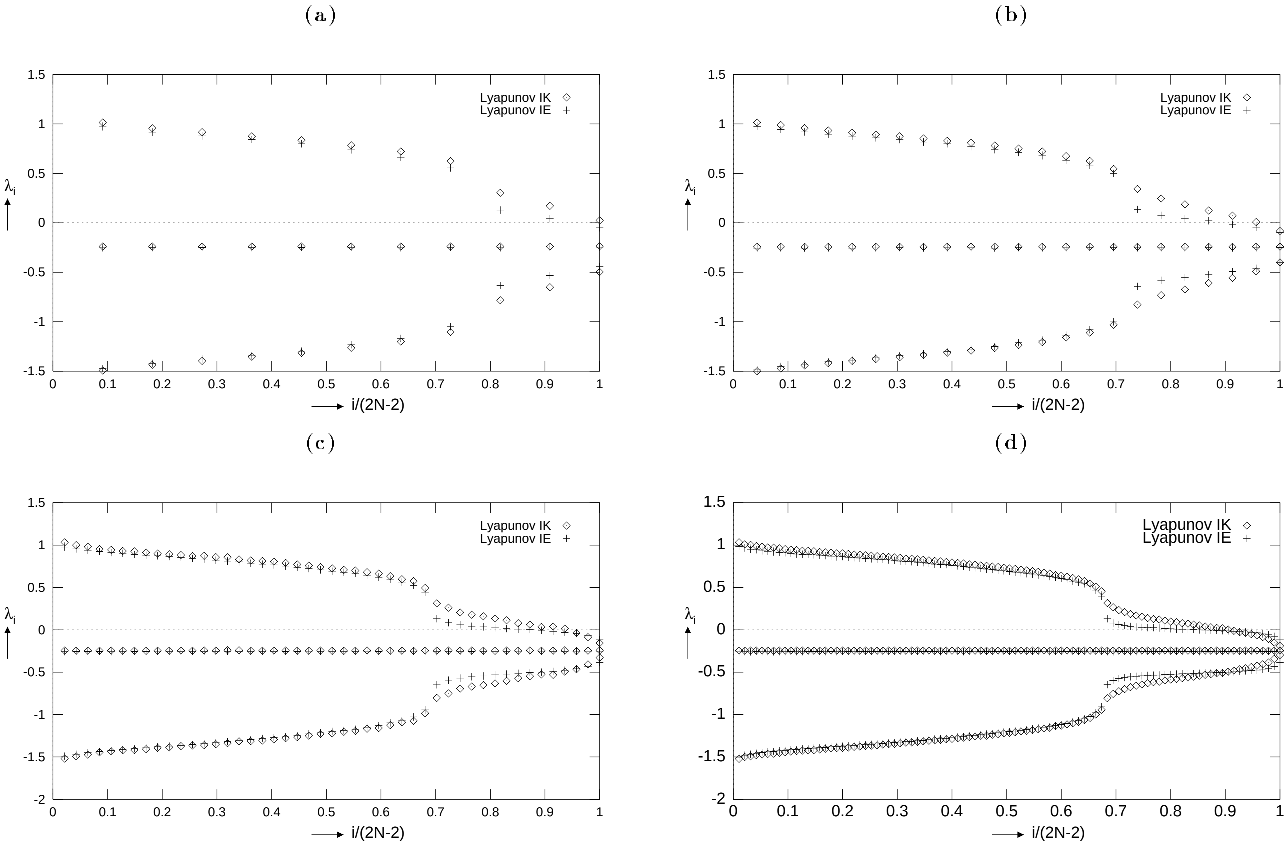

Fig. 9: Comparison of the Lyapunov spectrum λ_i of an IE system with the characteristic spectrum of an IK system associated with $\check{T}$ for (a) 4 particles; (b) 8 particles; (c) 16 particles; (d) 32 particles.

for any vectors $\mathbf{w}, \mathbf{w}' \in V_{\mathbf{x}}$. For more details we refer to Appendix A2.

3. To test the idea that for a large number of particles (i.e. in the thermodynamic limit) the IK and IE thermostats should give identical results we have done a number of simulations on a number of many particle Lorentz gases. The necessity to evaluate the full Lyapunov spectrum with high accuracy made it necessary to use high order integration methods leading to the impossibility of using a number of particles in excess of 32. In this setting we have considered also a different kind of thermostat (IPK) in which only the kinetic energy respect to the center of mass of the moving particles is constrined. The results of the simulations seem to be in good agreement with the hypothesis that pairing should hold (possibly in a strong sense) for IE and IPK systems in the thermodynamic limit. This hypothesis was first used heuristcally in [7]. However, as shown in section 4, it cannot easily be converted into a proof of CPR. Nevertheless, the numerical results obtained here are consistent with this hypothesis, thus suggesting an interesting property of large thermostatted Hamiltonian systems.

Acknowledgement

Two of us (FB and EGDC) gratefully acknowledge financial support by grant DE-FG02-88-ER13847 of the US Department of Energy, as well as from ESI in Vienna. One of us (F.B.)

is endebted to C. Liverani and M. Wojtkowski for helpful discussions at ESI. C.P. expresses his thanks to the Rockefeller University for support during 1996–1997. We also acknowledge helpful discussions with C. Dettmann.

A1. Hamiltonian equivalence

In [12] it was shown that an IK system for a given value of the energy can be mapped into a Hamiltonian system on an energy surface by a proper time rescaling and redefinition of the momenta. More generally it was shown in [2] that any α-symplectic dynamics can be mapped into a symplectic one ($\alpha = 0$) one. In [12] there is no explicit derivation of the proper rescaling, but it is quite easy to derive this starting from a Hamiltonian system. We note that if such a transformation to a Hamiltonian system can be found for an IE system, this will quite easily lead to a proof of SCPR. Moreover we believe that, if SCPR holds for an IE system, some kind of mapping into a Hamiltonian system should be possible[19]. To be general enough we consider a Hamiltonian H of the form eq.(1.1) with equations of motion given by eq.(1.2)(1.4).

We now try to find a function $t(\lambda)$ of some new time variable λsuch that $\frac{1}{2}\sum_i \vec{q}_i\,'(t(\lambda))^2 + \phi^{int}(\underline{q}) = \mathcal{E}$ for some constant $\mathcal{E}$ representing the new fixed internal energy. Here the prime represents the derivative respect to λ, *i.e.* $\vec{q}_i\,'(t(\lambda)) = d\vec{q}_i(t(\lambda))/d\lambda$. This leads, if we restrict ourself to the $H = E$ energy surface, to:

$$t'(\lambda)^2 = \frac{\mathcal{E} - \phi^{int}(\underline{q})}{E - \phi^{int}(\underline{q}) - \phi^{ext}(\underline{q})} \tag{A1.1}$$

Defining $\underline{\pi} = t'(\lambda)\underline{p}(t(\lambda))$ we get

$$\begin{cases} \vec{q}_i\,' = \vec{\pi}_i \\ \vec{\pi}_i\,' = \vec{F}_i^{ext}(\underline{q}) + \vec{f}_i^{int}(\underline{q}) - \alpha(\underline{\pi}, \underline{q})\vec{\pi}_i \\ \alpha(\underline{\pi}, \underline{q}) = \dfrac{\sum_i \vec{\pi}_i' \vec{F}_i^{ext}(\underline{q})}{\sum_i \vec{p}_i^2} \end{cases} \tag{A1.2}$$

where

$$\vec{F}_i^{ext}(\underline{q}) = \frac{(\mathcal{E} - \phi^{int}(\underline{q}))(\vec{f}_i^{ext}(\underline{q}) + \vec{f}_i^{int}(\underline{q}))}{E - \phi^{int}(\underline{q}) - \phi^{ext}(\underline{q})} - \vec{f}_i^{int}(\underline{q}) \tag{A1.3}$$

It is now easy to see that if we set $\phi^{int}(\underline{q}) = 0$ we obtain:

$$\vec{F}_i^{ext}(\underline{q}) = \mathcal{E}\frac{\vec{f}_i^{ext}(\underline{q})}{E - \phi^{ext}(\underline{q})} = \mathcal{E}\vec{\nabla}_i \log(E - \phi^{ext}(\underline{q})) \tag{A1.4}$$

which is exactly the inverse transformation of the one in [12].

The system (A1.3) looks very much like an IE system. The only problem is that the force $\vec{F}_i^{ext}(\underline{q})$ is not a gradient unless $\phi^{ext}(\underline{q})$ is a multiple of $\phi^{int}(\underline{q})$ [21]. This shows that it is, in general, not possible to map an IE system into a Hamiltonian system, at least using the simple mappings discussed here.

A2. A geometric condition for strong pairing

In general, for the thermostatted systems we are considering, the Lyapunov spectrum contains two zero exponents, one due to the presence of a constant of the motion (kinetic energy for IK, internal energy for IE and peculiar kinetic energy for IPK) and the other due to the motion in the time direction. To see whether the other Lyapunov exponent pair to a non zero value, one has to conceive a well defined procedure to split off the two zero exponents from the spectrum. This is done in [1] by a Poincaré section like procedure. We want to give here a general version of this procedure, leading to an explicit algebraic condition on the differential of the flow for having strongly paired Lyapunov exponents.

As a general setting we consider the phase space of our system as being a $2n-1$ sub-manifold Σ of R^{2n} (the full $(\underline{p},\underline{q})$ phase space) for some integer n defined by a particular level set of the constant of the motion (*i.e.* the set of points on which the constant of motiom takes a given value). The flow itself, denoted by φ_t, is generated by a vector field $\underline{\mathbf{v}}$, so that

$$\dot{\varphi}_t(\mathbf{x}) = \underline{\mathbf{v}}(\varphi_t(\mathbf{x})) \qquad (A2.1)$$

for $\mathbf{x} \in \Sigma$.

We will also consider in R^{2n} the standard symplectic matrix $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$, already defined in sect. 2, where I is the $n \times n$ identity matrix. It seems natural to introduce J considering that, both in the Hamiltonian and in the IK case pairing comes from symplectic properties of the flow φ_t. In general, we can consider Σ as a $2n-1$ submanifold of some more general symplectic manifold $\mathcal{M}$ but we will consider only the case $\mathcal{M} = R^{2n}$ with the symplectic structure given by J.

We now apply this to the pairing property. The Lyapunov spectrum of the flow φ_t, with φ_t defined only on Σ, does not contain the zero exponent due to the imposed constant of the motion. To eliminate also the second zero exponent in the time direction we proceed as follows, following [1]. At any point $\mathbf{x} \in \Sigma$ we consider an hyperplane $V_{\mathbf{x}}$ of R^{2n} at $\mathbf{x}$ and uniformely transversal to $\mathbf{v}_{\mathbf{x}}$, *i.e.* the angle between $V_{\mathbf{x}}$ and $\mathbf{v}_{\mathbf{x}}$ is everywhere bounded away from 0. The intersection between $V_{\mathbf{x}}$ and Σ defines a $(2n-2)$-dimensional submanifold $\Omega_{\mathbf{x}}$ whose tangent space $E_{\mathbf{x}}$ is just the intersection between the tangent space of Σ at $\mathbf{x}$, $T_{\mathbf{x}}\Sigma$, and $V_{\mathbf{x}}$ (here and in what follows we will identify R^{2n} with its tangent space at any point, so that $T_{\mathbf{x}}V_{\mathbf{x}} = V_{\mathbf{x}}$). Observe that the family $V_{\mathbf{x}}$ can be defined as the family of hyperplanes orthogonal to a vector field $\mathbf{g}_{\mathbf{x}}$ on Σ (in general $\mathbf{g}_{\mathbf{x}}$ need not be in $T_{\mathbf{x}}\Sigma$, it can be in R^{2n}, but in what follows we will always consider $\mathbf{g}_{\mathbf{x}} \in T_{\mathbf{x}}\Sigma$). The family $V_{\mathbf{x}}$ will allow us to define a new flow, Φ_t, whose Lyapunov spectrum will not contain the second zero exponent as well.

Given now a point $\mathbf{x}(0) \in \Sigma$ and its time evolved point $\mathbf{x}(t) = \varphi_t(\mathbf{x}(0))$ after a given time t, we can define a new map Φ_t from a neighborhood of $\mathbf{x}(0)$ in $\Omega_{\mathbf{x}(0)}$ to $\Omega_{\mathbf{x}(t)}$ as follows. Given a point $\mathbf{x}'(0) \in \Omega_{\mathbf{x}(0)}$ close enough to $\mathbf{x}(0)$, we consider the time $\tau(\mathbf{x}'(0), t)$ at wich the trajectory starting from $\mathbf{x}'(0)$ intersects $\Omega_{\mathbf{x}(t)}$. Here and in the following we suppress the dependence on $\mathbf{x}(0)$. Setting then $\Phi_t(\mathbf{x}'(0)) = \varphi_{\tau(\mathbf{x}'(0),t)}(\mathbf{x}'(0))$ it is clear that $\Phi_t(\mathbf{x})$ can be considered as a new flow and that its Lyapunov spectrum, *i.e.* the eigenvalues of $\Lambda = \lim_{t\to\infty} \frac{1}{2t} \log D\Phi_t^{tr} D\Phi_t$, are identical to those of φ_t at $\mathbf{x}(0)$, except that they do not contain the two zero exponents. Here $D\Phi_t : V_{\mathbf{x}(0)} \to V_{\mathbf{x}(t)}$ is the differential of Φ_t and is given in local coordinate by:

$$\big(D\Phi_t\big)_{i,j} = \frac{\partial(\Phi_t)_i}{\partial \mathbf{x}_j} \tag{A2.2}$$

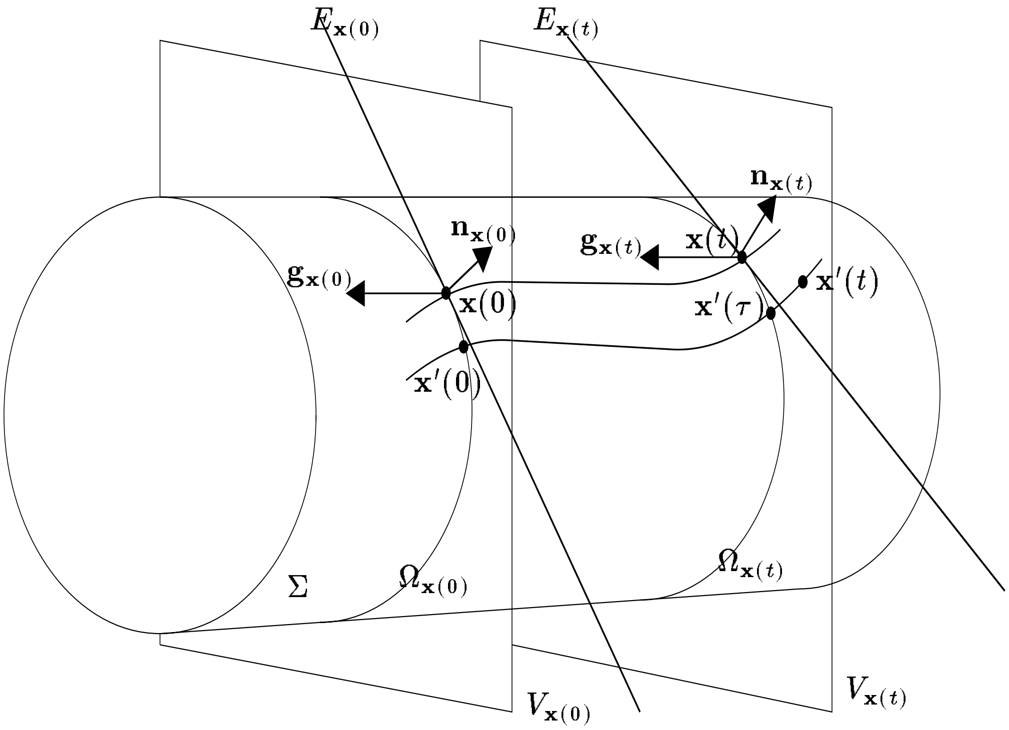

Fig. 10: Schematic representation of the construction of the flow Φ_t. Here $\mathbf{x}(t) = \varphi_t(\mathbf{x}(0))$, $\mathbf{x}'(t) = \varphi_t(\mathbf{x}'(0))$ and $\mathbf{x}'(\tau) = \Phi_t(\mathbf{x}'(0)) \in \Omega_{\mathbf{x}(t)}$. The other symbols are explained in the text.

Oberve that, calling $L_t = D\Phi_t$, we have $\dot{L}_t = T(\mathbf{x}(t))L_t$ where $T(\mathbf{x})$ is a matrix uniquely defined at every point $\mathbf{x}$ of Σ, independently of $\mathbf{x}(0)$, contrary to Φ_t and L_t. In fact we have:

$$T(\mathbf{x})_{i,j} = \frac{d}{dt}\big(D\Phi_t(\mathbf{x})\big)_{i,j} = \frac{d}{dt}\left(\frac{(\partial\varphi_\tau(\mathbf{x}))_i}{\partial\tau}\frac{\partial\tau(\mathbf{x},t)}{\partial\mathbf{x}_j} + \frac{(\partial\varphi_\tau(\mathbf{x}))_i}{\partial\mathbf{x}_j}\right) \tag{A2.3}$$

so that, for $\mathbf{w} \in E_{\mathbf{x}}$ one has, after straightforward algebraic manipulations:

$$T(\mathbf{x})\mathbf{w} = \left[\frac{d}{dt}(D\tau)\mathbf{w}\right]\mathbf{v}_{\mathbf{x}} + \left[(D\tau)\mathbf{w}\right]\frac{d}{dt}\mathbf{v}_{\mathbf{x}} + \frac{d}{dt}(D\varphi_t)\mathbf{w} \qquad (A2.4)$$

where $D\tau$ is the differential of τ with respect to $\mathbf{x}$.

Noting that $\frac{d}{dt}(D\varphi_t) = (D\mathbf{v})(D\varphi_t)$ we obtain:

$$T(\mathbf{x})\mathbf{w} = \left[\left(\frac{\partial D\tau}{\partial t}\mathbf{w}\right)\right]\mathbf{v} + (D\underline{\mathbf{v}})w \qquad (A2.5)$$

It is now easy to show that $\frac{\partial D\tau}{\partial t} = \mathbf{b} + \tilde{\mathbf{b}}$ with

$$\mathbf{b} = \frac{\dot{\mathbf{g}} + (D\mathbf{v})^{tr}\mathbf{g}}{(\mathbf{v}, \mathbf{g})} \qquad (A2.6)$$

and $\tilde{\mathbf{b}}||\mathbf{g}$. Moreover the component of the vector $\mathbf{b}$ along $V_{\mathbf{x}}$ is unique. Thus eq.(A2.5) can be written as:

$$T\mathbf{w} = (D\mathbf{v})\mathbf{w} + (\mathbf{b}, \mathbf{w})\mathbf{v} \qquad (A2.7)$$

where $\mathbf{w} \in E_{\mathbf{x}}$ and $\mathbf{b}$ is given by eq.(A2.6).

It is known, see [1] for a simple proof, that if for any $\mathbf{w}, \mathbf{w}' \in E_{\mathbf{x}_0}$

$$(L_t\mathbf{w}, JL_t\mathbf{w}') = \mu_t(\mathbf{w}, J\mathbf{w}') \qquad (A2.8)$$

where $\mu_t = \exp(\int_0^t \alpha(\mathbf{x}(\tau))d\tau)$ for some function $\alpha(\mathbf{x})$ defined on Σ, then if λ is in the spectrum of $\Lambda_t = L_t^{tr}L_t$, so is μ^2/λ. This immediately implies that if $\lim_{t\to\infty}\frac{1}{2t}\log\Lambda_t$ exists then its eigenvalues are strongly paired in the sense of sec. 1. Moreover, for any ergodic measure for φ_t the Lyapunov exponents of φ_t are paired. Observe that in order give meaning to eq.(A2.8) we need that $V_{\mathbf{x}}$ is a symplectic plane, *i.e.* $JV_{\mathbf{x}} = V_{\mathbf{x}}$. To achieve this we must set $\mathbf{g} = J\mathbf{n}$ where $\mathbf{n}$ is the normal vector to Σ at $\mathbf{x}$. We will say that L_t is α-symplectic if eq.(A2.8) holds. Moreover we will say that the flow φ_t is α-symplectic if for any $\mathbf{x}_0$ and for any t the matrix L_t is α-symplectic. We can now state the result.

Theorem A2.1: *The flow φ_t is α-symplectic if and only if for any $\mathbf{x} \in \Sigma$ and for all $w, w' \in E_{\mathbf{x}}$ the skew symmetric matrix $M = JT + T^{tr}J$ satisfies:*

$$(w, Mw') = \alpha(w, Jw') \qquad (A2.9)$$

where $\alpha : \Sigma \to R$ is a suitable function and T is given by eq.(A2.7).

Eq. (A2.9) follows immediately by differentiating eq.(A2.8) with respect to t.

Theorem A2.1 provides a well defined algebraic condition that can be easily checked in cases of interest. In fact, straightforward computation shows that it is indeed satisfied in the case of the IK dynamics studied by Dettmann and Morris in [1] as well as in the case of constant α, studied by Dressler in [8].

References.

[1] C.P. Dettmann, G.P. Morriss, "Proof of Lyapunov exponent pairing for system at constant kinetic energy", Phys. Rev E **53**, 5545-5548 (1996).

[2] M Wojtkoski, C. Liverani, "Conformally symplectic dynamics and symmetry of Lyapunov spectrum",Comm. Math. Phys. (1997) in print (Jan. 30).

[3] H.A. Posch, W.G. Hoover: "Lyapunov instability of dense Lenard-Jones fluids", Phys. Rev. A. **38**, 473–482 (1988).

[4] E.G.D. Cohen, L. Rondoni: "Note on phase space contraction and entropy production for thermostatted systems", archived in cond-mat@xxx.lanl.gov #9712213.

[5] D.J. Evans, G.P. Morris: *Statistical Mechanics of nonequilibrium fluids*, Accademic Press (1990).

[6] D.J. Searles, D.J. Evans, D.J. Isbister, "The conjugate pairing rule for non-Hamiltonian systems", Chaos, Focus issue on "Chaos and Irreversibility", (1998).

[7] D.J. Evans, E.G.D. Cohen, G.P. Morris, "Viscosity of a simple fluid from its maximal Lyapunov exponents", Phys. Rev. A **42** 5590–5597 (1990).

[8] U. Dressler, "Symmetry properties of the Lyapunov spectra of a class of dissipative dynamical systems with viscous damping", Phys. Rev. A **38**, 2103-2109 (1988).

[9] R. Zwanzig:"Time-Correlation Functions and Transport Coefficient in Statistical Mechanics", Ann. Rev. Phys. Chem. **16**, 67-102 (1965).

[10] D. Ruelle: "Positivity of entropy production in nonequilibrium statistical mechanics", in mp-arch@math.utexas.edu # 96-166.

[11] G. Gallavotti: "Chaotic hypothesis: Onsager reciprocity and fluctuation dissipation theorem", J. Stat. Phys. **84**, 899-926, (1996); ibid., "Extension of Onsager's reciprocity to large field and the chaotic hypothesis", Phys. Rev. Lett. **77**, 4334-4337, (1996); G. Gallavotti, D. Ruelle: "SRB states and nonequilibrium statistical mechanics close to equilibrium", in mp-arch@math.utexas.edu # 96-645, in print on Comm. Math. Phys..

[12] C.P. Dettmann, G.P. Morriss, "Hamiltonian formulation of the Gaussian Isokinetic Thermostat", Phys. Rev. E **54**, 2495-2500 (1996).

[13] N.I. Chernov, G.L. Eyink, J.L. Lebowitz, Ya.G. Sinai, "Steady state electric conduction in the periodic Lorentz gas", Comm. Math. Phys. **154**, 569–601 (1993).

[14] J.M. Eckmann, D. Ruelle,"Ergodic Theory of Chaos and Strange Attractors",Rev. Mod. Phys. **57** 617–656 (1985).

[15] G. Benettin, L. Galgani, A. Giorgilli,J.M. Strelcyn,"Tous les nombres charactéristiques de Lyapunov sont effectivement calculable", C. R. Acad. Sci. Paris, Ser A–B **286** A431–A433 (1978).

[16] R. Bowen, *Equilibrium states and the ergodic theory of Anosov diffeomorphism*, Lecture Notes in Mathematics **470**, Springer, Berlin (1975).

[17] F. Bonetto, G. Gallavotti, P.L. Garrido, "Chaotic Principle: an experimantal test", Physica D **105**, 226-252 (1997).

[18] H.A. Posch: "Lyapunov instability of the boundary-driven Chernov-Lebowitz model for stationary shear flow", J. Stat. Phys. **88** 825–842 (1997).

[19] M.J. Feigenbaum, Private communication.

[20] D.J. Evans, S. Sarman:"Equivalence of thermostatted nonlinear responses", Phys. Rev. E **48**, 65-70 (1993); G. Gallavotti "Equivalence of dynamical ensamble and Navier-Stokes equations", Phys. Rev. Lett. **223**, 91-95 (1996); ibid. "Dynamical Ensemble equivalence in Statistical Mechanics", Physica D, in print.

[21] The same observation was made independently by C. Dettmann.