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The brief time-reversibility of the local Lyapunov exponents for a small chaotic Hamiltonian system

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ABSTRACT

We consider the local (instantaneous) Lyapunov spectrum for a four-dimensional Hamiltonian system. Its *stable* periodic motion can be reversed for long times. Its *unstable* chaotic motion, with two symmetric pairs of exponents, cannot. In the latter case reversal occurs for more than a thousand fourth-order Runge–Kutta time steps, followed by a transition to a new set of paired Lyapunov exponents, unrelated to those seen in the forward time direction. The relation of the observed chaotic dynamics to the Second Law of Thermodynamics is discussed.

1. Introduction

All fundamental equations of classical physics could be described by a Hamiltonian form $\boldsymbol{H}(p_i,q_i)$ [1] with the equations of motion $\mathrm{d}q_i/\mathrm{d}t = \delta\boldsymbol{H}/\delta p_i$ and $\mathrm{d}p_i/\mathrm{d}t = -\delta\boldsymbol{H}/\delta q_i$. They are, in principle, all time reversible in contrast to the irreversibility of the Second Law of Thermodynamics [2]. Recently, the irreversibility of "large" Hamiltonian systems with thousands of degrees of freedom has been characterized in [3] by studying their chaotic motion. Indeed, for large chaotic systems their irreversibility is connected with the Second Law of Thermodynamics, see Lebowitz [4], Evans et al. [5], and Gallavotti et al. [6]. It is the aim of this paper to extend and contrast this research to the properties of the smallest-possible Hamiltonian system with chaotic behaviour, a simple four-dimensional model, although the Second Law of Thermodynamics is a property of the statistics of large macroscopic systems.

Before going into the details, some facts of chaos will be described in brief. Assume there is an n-dimensional solution $\underline{x}(t)$, called the trajectory, in the phase space $\boldsymbol{R}(\underline{x})$ evaluated from a set of n equations of motion $\mathrm{d}\underline{x}/\mathrm{d}t = \underline{X}(\underline{x})$. Their local instantaneous Jacobian matrix [7] is $\boldsymbol{J}(t) = \mathrm{d}\underline{X}(t)/\mathrm{d}\underline{x}(t)$. Note that for a Hamiltonian equation of motion the sum of the diagonal elements of $\boldsymbol{J}$ is zero, with symplectic as special case for zeros in all diagonal elements. Within the tangent space of $\underline{x}(t)$ an orthogonal frame $\boldsymbol{F}$ of n vectors $\underline{f}_i$ to neighbouring points is defined at the start. Following in the spirit of Benettin et al. [8], explaining their convergence by Ershov and Popatov [9], they are moving in time in first order by $\underline{f}_i(t+\mathrm{d}t) = \underline{f}_i(t) + \boldsymbol{J}(t)\underline{f}_i(t)\mathrm{d}t$. The first vector $\underline{f}_1$ will, after a transient time, point into the direction of extreme global expansion as shown by Oseledec [10]. The remaining directions will be orthogonalised after each time step by the Gram-Schmidt procedure [11] (or by Lagrange multipliers). The logarithm of local instantaneous expansion in the direction of $\underline{f}$ is the local Lyapunov [12] exponent $\lambda_{\underline{u}} = (\underline{u}, \boldsymbol{J}\underline{u})$, defined as scalar product if $\underline{f}$ is normalized to the unit vector $\underline{u}$, see [13]. The global asymptotic Lyapunov exponents are approximated by the average of the local exponents for long times. If the first global exponent is positive, the trajectory is chaotic.

2. Pairing symmetry and time-reversal symmetry

Before asking: "Is it possible to combine the pairing symmetry of the local exponents for Hamiltonian systems

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with time-reversal symmetry?", the frames for forward and backward motions will be described together with the pairing symmetry.

2.1. Forward motions

First, we describe the pairing symmetry [14–16] of Hamiltonian systems for n-dimensional chaotic problems. Any initial randomly chosen orthogonal frame $F_f(t_0)$ will be rotated, using the Gram-Schmidt algorithm, for forward time $t = t_f$ with positive time step dt_f by the equations of motion. At every time step dt_f the frame $F_f(t)$ is orthogonalised with the Gram-Schmidt procedure. After an initial transient period τ a transient frame $F_f = T_f$ converges well to the local unique frame $U_f(t)$. This frame is defined when for different initial frames $F_f(t_0)$ the same frame $U_f(t)$ results. The local Lyapunov exponents of the transient frame T_f have no pairing symmetry. For very complicated chaotic problems, as in [3], this transient time τ can be very long. It appears that using the equations of motion $dq_i/dt = \delta H/\delta p_i$ and $dp_i/dt = -\delta H/\delta q_i$, only the local exponents λ_i^{Uf} of the unique frame $U_f(t)$ have pairing symmetry

$$\lambda_i^{Uf}(t) = -\lambda_{n+1-i}^{Uf}(t)$$

2.2. Backward motions for time-reversal

Second, time reversal starts at a positive time t_s with time $t = t_b$ going backwards, using a negative time step dt_b. Instead of evaluating again the Lyapunov-unstable time-reversed trajectories, the stored trajectories of the forward motion or a bit-reversible algorithm can be used [17,18]. An initial random frame $F_b(t_s)$ will be followed backward in time with Gram-Schmidt orthogonalization. Again, during a transient time τ there is a transient frame T_b with no pairing symmetry. When finally the unique local backward frame $U_b(t)$ is approximated, there once again is pairing symmetry described by

$$\lambda_i^{Ub}(t) = -\lambda_{n+1-i}^{Ub}(t).$$

2.3. Time-reversal symmetry

To test for time-reversal symmetry, the exponents $\lambda_i^{Uf}(t)$ have to be compared to the same exponents $-\lambda_i^{Ub}(t)$ for the same time t, for $t = t_f$ obtained from 'below' (past), for $t = t_b$ from 'above' (future), at the coincidence $t_f = t_b$.

It is well established that for chaotic systems there is no time reversal symmetry for the properly-converged local exponents [4], thus

$$\lambda_i^{Uf}(t) \neq -\lambda_i^{Ub}(t).$$

Therefore, forward and backward pairing symmetries are different

$$\lambda_i^{Uf}(t) = -\lambda_{n+1-i}^{Uf}(t) \neq \lambda_i^{Ub}(t) = -\lambda_{n+1-i}^{Ub}(t).$$

2.4. Covariant Lyapunov vectors not suited to simulate laboratory experiments or adequate simulations

Since, for chaos, there are two different local frames $U_f(t)$ and $U_b(t)$, is seems appropriate to combine them to a single local frame resulting in mathematically defined covariant Lyapunov vectors (CLV) being non-orthogonal, see [19,20], and the references cited therein. A disadvantage of the covariant vectors is that the exponents associated with them are not simply related to the change of phase volume. Further, transients after the time-reversal are considered to be non-interesting, only the later convergent patterns are used to define the CLV. In addition, similar to the Gram-Schmidt vectors and their exponents, CLVs are scale dependent [21], they are not fully universal.

However, both strongly nonequilibrium physical experiments and faithful simulations of them can only be carried out forward in time. Similarly, backward analysis should not be mixed with forward analysis. Further, we apply the standard method to evaluate Lyapunov exponents with orthogonal frames. We will compare the results of backward to forward, but not combining them to a different feature. In sum, we consider CLV not suitable to treat physical problems, which are never a combination of forward and backward. Finally, we are interested in the transient behaviour just after the time reversal. If short transients of time-reversal are found, we ask why they are so short.

2.5. Time reversal starting with forward frame: both short pairing and time reversal symmetry for chaos

There is a further question involving reversibility. Consider using the local stable frame $U_f(t_s)$ rather than random initial conditions at the time t_s of time reversal. Then, backwards, only the sequence of the directions for the orthogonalization is reversed, thus backward 4321 instead of forward 1234, i.e. the first is orthogonalised last, but keeps number 1. Indeed, though at present only tested for relatively small-dimensional Hamiltonian systems, there is a relatively short time for which the frame U_b is the same as U_f. This implies full time-reversal symmetry of the exponents, combined with pairing symmetry. There is a sign change for the exponents since expanding and contracting directions are exchanged. An algebraic proof of that sign change is given in Appendix B as written by a reviewer.

$$\lambda_i^{Uf}(t) = -\lambda_{n+1-i}^{Uf}(t) = -\lambda_i^{Ub}(t) = \lambda_{n+1-i}^{Ub}(t).$$

Considering the behaviour just after the time reversal performed in the above way. There is a combination of pairing symmetry and time-reversal symmetry, however, only for a small time interval. This symmetry is unstable in all of the chaotic cases we have examined with a non-perfect algorithm. It is destroyed by fluctuations. The time for this destruction is dependent on the strength of chaos, the number n of the dimensions, and the accuracy of the integration process related to the magnitude of the time steps.

2.6. Infinite pairing and time reversal symmetry for non-chaos movements

Further, without chaos (as in a stable periodic orbit) there is both pairing and time-reversal symmetry for all times, evaluated with the same non-perfect algorithm as the chaos problem. This shows that, in principle, the Gram-Schmidt procedure is reversible. In addition to that numerical argument, a reviewer has designed an algebraic