Proof of Lyapunov Exponent Pairing for Systems at Constant Kinetic Energy

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(Phys. Rev. E, **53**, R5545 (1996))

We present a proof that a system consisting of any finite number of particles, which move under the action of a scalar potential at constant kinetic energy exhibits conjugate pairing of Lyapunov exponents, that is, the Lyapunov exponents come in pairs, which sum to the same constant. This result generalizes previous results, because it is independent of the size of the system.

PACS: 05.45.+b 05.70.Ln

The conjugate pairing rule states that a trajectory which has a given Lyapunov exponent λ also has an exponent $C-\lambda$, where C is a constant which depends on the trajectory, but is the same for all pairs of exponents. Hamiltonian systems obey this rule for all trajectories, with $C=0$, that is, the exponents come in $\pm$ pairs [1]. The other general class of such systems are those with a constant damping factor [2], for which C is proportional to this factor. There is numerical evidence [3–5] for conjugate pairing in thermostatted systems (below), as well as arguments for the case of a large number of particles [6]

Thermostatted systems are important in the study of nonequilibrium molecular dynamics (NEMD) simulations. NEMD calculations evaluate transport coefficients by considering a large number of particles subject to both interparticle forces and an external field, which drives the system into a nonequilibrium state. The use of an extra ("thermostatting") term in the equations permits the system to be stationary in time and homogeneous in space by removing excess energy generated by the external field. The alternative is to simulate nonequilibrium effects via boundary conditions, at the expense of homogeneity. It can be shown that the transport coefficients derived from thermostatted NEMD calculations are equivalent to those obtained from Green-Kubo formulae using equilibrium simulations [7].

The conjugate pairing rule permits the evaluation of the sum of all the Lyapunov exponents from the largest and smallest, which are the easiest to calculate. The sum of the exponents is significant because it is directly related to a macroscopic transport coefficient (such as the conductivity) in these systems [8].

The main result to date has been an argument that a thermostatted Hamiltonian system obeys conjugate pairing approximately, with errors inversely proportional to the number of degrees of freedom of the system [6]. This result ignores terms of order $1/N$ in the stability matrix and leaves open, therefore, the influence of these terms on its eigenvalues and consequently on conjugate pairing. For further discussion refer to Ref. [9]. Recently we have shown numerically that a system with the minimum number of pairs (two) exhibits conjugate pairing [10], thus suggesting that the size of the system may not be relevant. The present paper proves the result exactly for a restricted case, that is, isokinetic thermostats and forces derivable from a potential ϕ, for any value of N.

There is an important difference between the present result and past statements of the conjugate pairing rule in that here, we explicitly single out two trivial exponents (equal to zero) which do not pair. These are due to the conservation of kinetic energy, and time translation symmetry. They sum to zero, and so should not be included with the other pairs of exponents, which sum to another constant. Thus, the stability matrix (T, Eq. (22) below) does not satisfy Eq. (23) in the full $6N$-dimensional space, explaining the fact that previous calculations of T contained corrections, which happened to be of order $1/N$. We circumvent this problem by defining T for a reduced, $6N-2$-dimensional space, which specifically excludes perturbations which alter the kinetic energy, or are along the flow. In this space, pairing appears exactly.

Consider a system with equations of motion

$$\dot{\mathbf{x}} = \mathbf{p} \tag{1}$$

$$\dot{\mathbf{p}} = -\nabla\phi - \alpha\mathbf{p} \ . \tag{2}$$

Here, $\mathbf{x}$ is a $3N$-dimensional vector, containing the positions of N particles multiplied by the square-root of their masses, $\mathbf{p}$ is a vector constructed from the momenta divided by the square-root of the masses, and ϕ contains both interparticle potentials and external potentials. The scalar product of vectors generalizes in the natural way. This calculation is written in three dimensional language, but generalizes trivially to other dimensions.

To keep the total kinetic energy $\mathbf{p}\cdot\mathbf{p}/2$ constant, we have

$$\alpha = -\frac{\mathbf{p}\cdot\nabla\phi}{\mathbf{p}\cdot\mathbf{p}} \ , \tag{3}$$

hence the designation "isokinetic". Another common type of thermostat is called isoenergetic, where the kinetic plus interparticle potential energy is kept constant. Thermostats which constrain the energy instantaneously in this way are discussed with regard to Lyapunov exponents in Refs. [9,11]. There are also Nosé-Hoover thermostats [12–14], which also constrain the energy, but only in an average sense. The result presented here applies only to the isokinetic thermostat.

It is sometimes convenient to group together $\mathbf{x}$ and $\mathbf{p}$ to form a phase space point $\mathbf{X}$. There are two time dependent matrices used to describe the evolution of a linear perturbation $\delta\mathbf{X}$. They depend on the phase space point $\mathbf{X}$, but this dependence will be suppressed for clarity. They are the infinitesimal and finite evolution matrices, T and L, respectively, defined by

$$\delta\dot{\mathbf{X}}(t) = T(t)\delta\mathbf{X}(t) \ , \tag{4}$$

$$\delta\mathbf{X}(t) = L(t)\delta\mathbf{X}(0) \ . \tag{5}$$

The matrix T is usually obtained by differentiating the equations of motion, however, we will evaluate it in a restricted subspace of the tangent space, which is slightly more complicated. L can be obtained from T as the solution of

$$\dot{L}(t) = T(t)L(t) \ , \tag{6}$$

$$L(0) = I \ . \tag{7}$$

The Lyapunov exponents are defined as the logarithms of the eigenvalues of Λ, where

$$\Lambda = \lim_{t\to\infty} \left(L^T(t)L(t)\right)^{1/(2t)} \ . \tag{8}$$

Two of the Lyapunov exponents of the above thermostatted system are automatically zero, corresponding to perturbations along the evolution of the flow, which effectively add a constant to the time, and in the direction of increasing kinetic energy, which effectively multiply the time by a constant. We ignore these exponents for the purpose of the conjugate pairing rule, by effectively considering only those perturbations which are perpendicular to these directions. To be precise, we choose $6N-2$ perturbations, which are perpendicular to the direction of increasing kinetic energy, and none of which are exactly along the flow.

The basis vectors which are used to obtain components of $\delta\mathbf{X}$ rotate with the motion of the trajectory, so as to be always perpendicular to the direction of increasing kinetic energy. This means that the finite time eigenvalues may be different to those obtained with fixed basis vectors, but in the long time limit the results are the same. To see this, note that the Lyapunov exponents do not depend on the initial time. Choose an initial time such that the set of tangent vectors are close to a point of accumulation, to which they pass arbitrarily close an infinite number of times. Because the space of unit tangent vectors is compact, this is always possible. Then we have a situation in which the initial and final points on the trajectory are measured with respect to the same basis. This argument is also required in general relativity, in which it is not possible in principle to compare bases at two different points [15].

It is clear that a perturbation which preserves the kinetic energy at some initial time will continue to do so. This reduces the phase space to $6N-1$ dimensions. We introduce $6N-2$ orthonormal basis vectors, none of which are exactly along the flow, and demand that a perturbation $\delta\mathbf{X}$ be in the space spanned by these vectors. This effectively means that we are taking a Poincare section, and considering the perturbed point to be the one at which the perturbed trajectory intersects with the $6N-2$ dimensional space spanned by the vectors. This intersection is possible because the effective phase space has $6N-1$ dimensions due to the conservation of kinetic energy, so a line and a $6N-2$ dimensional space may be expected to intersect; it is guaranteed by the stipulation that the perturbations not be along the flow. In general, the time elapsed along the perturbed trajectory, t' runs at an infinitesimally different rate to t. It is straightforward to show that the Lyapunov exponents obtained using the reduced basis are the same as those in the full phase space, with the exception of the two zeros.

Without further ado let us calculate the infinitesimal evolution matrix T in the restricted $6N-2$ dimensional space. Let us scale the time so that $\mathbf{p}\cdot\mathbf{p}=1$, and one unit vector in $3N$-space is $\mathbf{e}_0=\mathbf{p}$. At time $t=0$, arbitrarily choose $3N-1$ unit vectors $\mathbf{e}_i$ which together with $\mathbf{e}_0$ form an orthonormal set. These vectors are used separately in both position and momentum space to form the required basis. This separation of phase space into position and momentum space, while retaining the canonically conjugate structure is what makes this proof possible, and singles out the isokinetic thermostat as being particularly tractable analytically. The perturbations are taken from the $6N-2$ dimensional subspace defined by the $\mathbf{e}_i$. This means that the two conditions required in the preceding paragraph are met, that is, no perturbations are in the direction of increasing kinetic energy (which corresponds to $\mathbf{e}_0$ in momentum space), and none are directly along the flow (which contains a component of $\mathbf{e}_0$ in position space). Now, the equations of motion may be written in the full ($6N$ dimensional) space as

$$\dot{\mathbf{x}} = \mathbf{p} \tag{9}$$

$$\dot{\mathbf{p}} = \dot{\mathbf{e}}_0 = \sum_i \mathbf{f}\cdot\mathbf{e}_i\mathbf{e}_i \tag{10}$$

where $\mathbf{f}=-\nabla\phi$, and i sums from 1 to $3N-1$, as it will throughout this paper. If we choose, for convenience, the unit vectors to have equations of motion

$$\dot{\mathbf{e}}_i = -\mathbf{f}\cdot\mathbf{e}_i\mathbf{e}_0 \tag{11}$$

then the time derivatives of $\mathbf{e}_\mu\cdot\mathbf{e}_\nu$ are automatically zero (μ and ν run from 0 to $3N-1$), so that the $\mathbf{e}_\mu$ remain an orthonormal basis. In more geometrical terms, the basis vectors are parallel transported along the trajectory (see Fig. 1).

We write the perturbed trajectory as

$$\mathbf{x}' = \mathbf{x} + \sum_i \delta x_i\mathbf{e}_i \tag{12}$$

$$\mathbf{p}' = \mathbf{p} + \sum_i \delta p_i\mathbf{e}_i \ , \tag{13}$$

with equations of motion

$$\frac{d}{dt'}\mathbf{x}' = \mathbf{p}' \tag{14}$$

$$\frac{d}{dt'}\mathbf{p}' = \sum_i \mathbf{f}' \cdot \mathbf{e}_i' \mathbf{e}_i' \quad . \tag{15}$$

Here, $\mathbf{f}'$ is the value of $\mathbf{f}$ at the new coordinates, and $\mathbf{e}_i'$ are new (arbitrary) unit vectors perpendicular to $\mathbf{p}'$. We have:

$$\mathbf{f}' = \mathbf{f} + \sum_i \delta x_i \nabla_i \mathbf{f} \quad , \tag{16}$$

and we choose the orthonormal set ($i = 1 \ldots 3N-1$):

$$\mathbf{e}_0' = \mathbf{p}' \tag{17}$$

$$\mathbf{e}_i' = \mathbf{e}_i - \delta p_i \mathbf{e}_0 \quad . \tag{18}$$

Substituting Eqs. (12,13,16,18) into Eqs. (14,15), ignoring quadratic perturbations, simplifying with the help of Eqs. (9-11), and taking components in the directions of the $\mathbf{e}_\mu$, we obtain $6N$ equations. One of these is not independent of the others, due to the conservation of the kinetic energy. One equation gives the relation between t' and t, and the remaining $6N-2$ determine the evolution of the perturbations:

$$\frac{dt}{dt'} = 1 + \sum_i \mathbf{f} \cdot \mathbf{e}_i \delta x_i \tag{19}$$

$$\delta \dot{x}_i = \delta p_i \tag{20}$$

$$\delta \dot{p}_i = \sum_j (-\nabla_i \nabla_j \phi - \mathbf{f} \cdot \mathbf{e}_i \mathbf{f} \cdot \mathbf{e}_j) \delta x_j - \mathbf{f} \cdot \mathbf{e}_0 \delta p_i \quad , \tag{21}$$

and note that $\mathbf{f} \cdot \mathbf{e}_0$ is the α defined in Eq. (3). From these equations, the infinitesimal evolution matrix may be read off as

$$T = \begin{pmatrix} 0 & I \\ M & -\alpha I \end{pmatrix} \quad , \tag{22}$$

where each of the elements are $(3N-1) \times (3N-1)$ submatrices. M is symmetric, and 0 and I are the zero and unit matrices, respectively. It is easy to check that T satisfies the equation

$$T^T J + J T = -\alpha J \quad , \tag{23}$$

where J is given by

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \quad . \tag{24}$$

We call Eq. (23) the "infinitesimally α-symplectic" condition. See also chapter 2 of Ref. [16]. In order to obtain the corresponding equation for L we consider $K = L^T J L$. Using Eqs. (6,23) we find that $\dot{K} = \dot{L}^T J L + L^T J \dot{L} = L^T T^T J L + L^T J T L = -\alpha L^T J L = -\alpha K$. Also, by Eq. (7), $K(0) = J$. Solving the equation for K, we find that L satisfies the "global μ-symplectic condition",

$$\mu L^T J L = J \quad , \tag{25}$$

where $\mu = \exp\left(\int_0^t \alpha(s) ds\right)$. To obtain the Lyapunov exponents, one uses Eq. (8) and considers

$$\mu^2 L^T L J L^T L = J \quad , \tag{26}$$

which follows from Eq. (25).

Now consider the eigenvalues of a matrix M which satisfies the equation $aM^T J M = J$ for some a. If λ is an eigenvalue, then $(\lambda a)^{-1}$ is also an eigenvalue. For

$$\det(M - \lambda I) = 0 \tag{27}$$

$$\Rightarrow \det((\lambda a)^{-1} I - M) = 0 \quad , \tag{28}$$

using the fact that the determinant of a product is the product of determinants, and the determinant of a transpose is equal to the original determinant. This last result is called the μ-symplectic eigenvalue theorem, and implies that the logarithms of the eigenvalues of M satisfy the conjugate pairing rule.

Applying this result to the current situation, with $a = \mu^2$ and $M = L^T L$, we find that the sum of a pair of the logarithm of the eigenvalues of $L^T L$ is

$$\ln \lambda + \ln((\mu^2 \lambda)^{-1} = -2 \int_0^t \alpha(s) ds \quad , \tag{29}$$

which is clearly independent of which pair of eigenvalues we chose. At this point we have a result which applies to any trajectory segment, no matter how small, if the above co-moving basis is used. Using the traditional (fixed) basis, we can only make a statement about the infinite time limit.

Finally, we take the $t \to \infty$ limit, and use Eq. (8). The result is that any pair of Lyapunov exponents (except the trivial zeros) sum to minus the time average of α.

An important corollary is that, if there is an invariance in the equations of motion leading to a zero exponent, the conjugate exponent is not zero as in the Hamiltonian case, but $- < \alpha >_t$. For example, consider the case of a single particle, where ϕ is independent of z. The system is invariant under a translation in the z direction, giving it one zero Lyapunov exponent. The equation for p_z is

$$\dot{p}_z = -\alpha p_z \quad , \tag{30}$$

which is clearly responsible for an exponent of $- < \alpha >_t$ for perturbations in this direction.

This proof is valid for any number of particles moving in a potential which may contain both external terms and interactions between the particles. The natural generalization of this result would be to other Hamiltonian systems and thermostats, as argued in Ref. [6] and/or SLLOD dynamics, in which conjugate pairing has been observed numerically [3]. Work is now proceeding in this direction.

We would like to thank E. G. D. Cohen for a careful reading of the manuscript, and L. Rondoni for helpful discussions.

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FIG. 1. The basis vectors for one particle in three dimensions are parallel transported along the trajectory. Refer to Eq. (11)