Journal of Statistical Physics, Vol. 74, Nos. 5/6, 1994

Symmetry of Lyapunov Spectrum

D. Gupalo,[1] A. S. Kaganovich,[1] and E. G. D. Cohen[1]

Received June 25, 1993

The symmetry of the spectrum of Lyapunov exponents provides a useful quantitative connection between properties of dynamical systems consisting of N interacting particles coupled to a thermostat, and nonequilibrium statistical mechanics. We obtain here sufficient conditions for this symmetry and analyze the structure of $1/N$ corrections ignored in previous studies. The relation of the Lyapunov spectrum symmetry with some other symmetries of dynamical systems is discussed.

KEY WORDS: Stationary fluid motion; nonequilibrium molecular dynamics; dynamical systems; Lyapunov exponents; Gaussian thermostat.

1. INTRODUCTION

Many important dynamical quantities are expressed in terms of characteristic or Lyapunov exponents (LE), which are rates of exponential growth of separation of initially close phase trajectories. There exist several algorithms to calculate LE,[1,2] but the more degrees of freedom the system has, the more time-consuming the computation procedure is. Therefore, it is extremely important that some physical systems have a symmetric Lyapunov spectrum (SLS). It is well known that Hamiltonian systems have an SLS with respect to zero due to their underlying symplectic structure.[3] For a system of anharmonic oscillators with a constant friction a similar symmetry was noted with respect to half the friction coefficient.[4]

In recent publications[7-9] an SLS associated with the equations of motion of a many-particle system representing a nonequilibrium stationary fluid motion was discovered (see also refs. 5 and 6). In that case, the symmetry property was established analytically only for large systems,[7] i.e., when terms of order 1, compared to those of order N, the number of

[1] Rockefeller University, New York, New York 10021.

particles in the system, were neglected, although computer simulations for $N = 4$ and even 2 also showed a symmetric Lyapunov spectrum, within the experimental accuracy.[9] These results also raised the following questions: What properties of the equations of motion lead to an SLS? Is this symmetry only an asymptotic property for large systems, and if so, can one then give an estimate of the error for finite systems? In the present study we try to answer these questions as generally as possible.

The paper is organized as follows. In Section 2 we introduce some useful definitions and review previously known results about systems having an SLS. Section 3 is devoted to a derivation of useful sufficient conditions for an SLS. In Section 4 we find the general form of the equations of motion for thermostatted systems. Thermostat coupling terms have to be added to the adiabatic equations of motion for a stationary state to exist, because, without a coupling to a heat bath the temperature of the system will rise indefinitely due to the continuous work done on the system by the external forces. The results we report are that if the adiabatic system is Hamiltonian with a short-range interaction potential and some additional restrictions are satisfied, then the thermostatted system has an SLS as an asymptotic property when $N \to \infty$, and the correction terms are of the order of $1/N$. We also analyze the structure of the $1/N$ corrections to the symmetry constant. In Section 5 we consider as an example the color conductivity algorithm designed to simulate self-diffusion under the effect of a constant external field. The symmetry constant is proportional to the time-averaged thermostat coupling multiplier for any number of particles in this case.

Finally, we summarize our results, and discuss the relation of SLS to other symmetries of dynamical systems and the connection between SLS and nonequilibrium statistical mechanics.

2. DEFINITIONS AND OUTLINE OF PREVIOUS WORK

Consider a dynamical system described by a set of equations

$$\begin{aligned} \dot{\mathbf{q}} &= \mathbf{f}(\mathbf{q}, \mathbf{p}, t) \\ \dot{\mathbf{p}} &= \mathbf{g}(\mathbf{q}, \mathbf{p}, t) \end{aligned} \tag{1}$$

where the components of the n-dimensional vectors $\mathbf{q}$ and $\mathbf{p}$ consist of the coordinates $\mathbf{q}_i$ and momenta $\mathbf{p}_i$, respectively, of the N d-dimensional particles of the system. In terms of phase space variables $\boldsymbol{\Gamma}$ these equations may be written as

$$\dot{\boldsymbol{\Gamma}} = \mathbf{G}(\boldsymbol{\Gamma}, t) \tag{2}$$

with initial conditions

$$\mathbf{\Gamma}(0) = \mathbf{\Gamma}_0 \tag{3}$$

We represent the solution of (2)–(3) in the form of a phase flow

$$\phi^t(\mathbf{\Gamma}_0) = \mathbf{\Gamma}(t), \qquad t \in [0, \infty) \tag{4}$$

Suppose $\mathbf{G}(\mathbf{\Gamma}, t)$ and its first derivatives are continuous functions and $\partial\mathbf{G}/\partial\mathbf{\Gamma}$ is bounded on the solution (4); then we can define the local stability matrix

$$A(\mathbf{\Gamma}, t) = \left\| \frac{\partial \mathbf{G}(\mathbf{\Gamma}, t)}{\partial \mathbf{\Gamma}} \right\| \tag{5}$$

and the evolution matrix

$$S^t_{\mathbf{\Gamma}_0} = \left\| \frac{\partial \phi^t(\mathbf{\Gamma}_0)}{\partial \mathbf{\Gamma}_0} \right\| = T\exp \int_0^t A(\mathbf{\Gamma}(\tau), \tau)\, d\tau \tag{6}$$

$T\exp$ indicates a time-ordered exponential with the latest times to the left, which can be written explicitly as

$$S^t_{\mathbf{\Gamma}_0} = \lim_{\varepsilon \to 0} \prod_{j=0}^{t/\varepsilon} e^{\varepsilon A(\mathbf{\Gamma}(t - j\varepsilon), t - j\varepsilon)} \tag{7}$$

The Lyapunov exponents (LE) are defined by[10]

$$\lambda_i = \ln \mu_i \tag{8}$$

where the $\{\mu_i\}$ are the eigenvalues of the symmetric positive-definite global stability matrix:

$$M_{\mathbf{\Gamma}_0} = \lim_{t \to \infty} [(S^t_{\mathbf{\Gamma}_0})^T S^t_{\mathbf{\Gamma}_0}]^{1/2t} \tag{9}$$

The SLS property is best known for Hamiltonian systems.[3] The local stability matrix of Hamiltonian systems consisting of N particles is composed of four $n \times n$ $(n = Nd)$ blocks with one diagonal block equal to minus the transpose of the other one and symmetric off-diagonal blocks. As a consequence of this block structure the infinitesimally symplectic condition holds:

$$A^T J + JA = 0 \tag{10}$$

where J is the simplest antisymmetric matrix:

$$J=\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{11}$$

with I and 0 the $n \times n$ identity and null matrices, respectively.

The global symplectic condition

$$S^T J S = J \tag{12}$$

follows then from the local condition (10) and definition (6). The SLS property with respect to zero is a consequence of the global condition (12) and definition (9)[3]

$$\lambda_i + \lambda_{2n+1-i} = 0, \qquad i = 1,..., n \tag{13}$$

Another important case is a Hamiltonian system with uniform damping described by the following equations[4]:

$$\begin{aligned} \dot{\mathbf{q}} &= \frac{\partial H}{\partial \mathbf{p}} \\ \dot{\mathbf{p}} &= -\frac{\partial H}{\partial \mathbf{q}} - \alpha \mathbf{p} \end{aligned} \tag{14}$$

where α is a positive constant. It can be formally reduced to a Hamiltonian system without damping by means of the transformation[11]

$$\tilde{\mathbf{q}} = \mathbf{q}, \qquad \tilde{\mathbf{p}} = \mathbf{p}e^{\alpha t}, \qquad \tilde{H} = He^{\alpha t} \tag{15}$$

The local condition (10) in this case is generalized to[4]

$$A^T J + JA = -\alpha J \tag{16}$$

and leads to the generalized global symplectic condition

$$S^T J S = e^{-\alpha t} J \tag{17}$$

which in turn leads to an SLS with respect to $-\alpha/2$:

$$\lambda_i + \lambda_{2n+1-i} = -\alpha, \qquad i = 1,..., n \tag{18}$$

The sum of the LE in the equations (13) or (18) can be related to average local features. Indeed, eigenvalues of $A(\Gamma, t)$ show the rates of deviation of two initially infinitesimally close trajectories along the directions of corresponding eigenvectors. The sum of all local eigenvalues (equal to the trace of A) is the instant rate of the phase volume growth in the infinitesimally small area around the given phase point. The sum of all LE is the mean rate of the phase volume growth as it evolves under the dynamics; therefore it is an average of the instant rates. Thus the sum of all LE should be equal to the trace of A averaged along the solution of (2). Now we formally derive this relationship using (8), (9), and (7):

$$\sum_{i=1}^{2n} \lambda_i = \ln \det M = \overline{\operatorname{tr} A} \overset{\text{def}}{=} \lim_{t \to \infty} \frac{1}{t} \int_0^t \operatorname{tr} A(\Gamma(\tau), \tau)\, d\tau \tag{19}$$

From (19) and (18) we see that for a system with an SLS property with respect to α there is the following connection between the symmetry constant α and the trace of the local stability matrix:

$$\alpha = \frac{\overline{\operatorname{tr} A}}{2n} \tag{20}$$

If our system is ergodic, the time average over the phase flow (4) designated by the bar is equal to the phase space average. The practical use of the condition (20) was demonstrated in ref. 12 on a few examples.

3. SUFFICIENT CONDITION FOR THE LOCAL STABILITY MATRIX

It is possible to derive n necessary and sufficient conditions on the global stability matrix M for the existence of an SLS in a variety of ways. However, all those conditions involve either the reflexive property of the characteristic polynomial of M,[3] or properties of traces of powers of M,[12] both of which use explicit solutions of the equations of motion. These n conditions can also be expressed in terms of the local stability matrix A, but only the relation (19) between the determinant of M and the time average of the trace of A over the trajectory yields a simple necessary condition (20). However, other useful sufficient conditions can be obtained following ideas used in the symplectic case.[3]

In order to do this it is convenient to introduce the matrix

$$L(t) = M^{2t} = S^T(t)\, S(t) \tag{21}$$

with eigenvalues $\{\nu_i(t)\}$. It follows from (8) that

$$\lambda_i = \lim_{t \to \infty} \frac{\ln \nu_i(t)}{2t} \tag{22}$$

A symmetric Lyapunov spectrum (13) around zero is equivalent to

$$\lim_{t \to \infty} [v_i(t)\, v_{2n+1-i}(t)]^{1/(2t)} = 1, \qquad i = 1,..., n \tag{23}$$

To transform this condition on the global variables into a sufficient condition on the local variables, we require that the matrices L and L^{-1} have the same Jordan form, since (23) then holds automatically. For this it is necessary and sufficient that there exists a nonsingular matrix P such that $L = PL^{-1}P^{-1}$. We further require the matrix P to be the same for all times t:

$$S^T(t)\, S(t)\, PS^T(t)\, S(t) = P \tag{24}$$

The system of sufficient conditions for (24) is then

$$\begin{aligned} S^T(t)\, PS(t) &= P \\ S(t)\, PS^T(t) &= P \end{aligned} \tag{25}$$

We note that for the special case $P = J$ the first equation in (25) is the global symplectic condition.[3] It is easy to show that the second equation in (25) is then redundant due to the property $J^2 = -I$.

To get a sufficient condition for the first equation in (25) in terms of the local stability matrix we use the definition (7) of the matrix S to obtain

$$\lim_{\varepsilon \to 0} e^{\varepsilon A^T(\Gamma(t), t)} P e^{\varepsilon A(\Gamma(t), t)} = P \tag{26}$$

Expanding the left-hand side of (26) in the powers of ε, we obtain to $O(\varepsilon)$

$$A^T(\Gamma(t), t)\, P + PA(\Gamma(t), t) = 0 \tag{27}$$

A particular case of (27) is the infinitesimally symplectic condition,[3] which could be obtained from (27) by setting $P = J$. The condition (27) is not only necessary, but also sufficient for (26). This can be readily seen by expanding the left-hand side of (26) in powers of ε and using (27).

Similarly, from the second condition in (25) one obtains another condition on the local stability matrix:

$$A(\Gamma(t), t)\, P + PA^T(\Gamma(t), t) = 0 \tag{28}$$

Equations (27) and (28) give the sufficient conditions on the local stability matrix for an SLS. Once again for $P = J$ the second condition is redundant.

It has been shown[12] that a physical system having an SLS with respect to $-\alpha/2$ with $\alpha > 0$ can be derived from a system with an SLS property with respect to zero by an exponential dilation of the phase space coordinates which leads to $-(\alpha/2)\,I$ being added to the local stability matrix, to the evolution matrix multiplied by $e^{-(\alpha/2)t}$, and all LE being shifted by $-\alpha/2$. This approach can be generalized even further.[7] If $-\frac{1}{2}\alpha(\Gamma, t)\,I$ is added to the local stability matrix of the system with an SLS with respect to zero, then the new system would have an SLS with respect to $-\bar{\alpha}/2$, where the averaging is in the same sense as in Eq. (19).

Thus, substituting $A + \frac{1}{2}\alpha(\Gamma, t)\,I$ for A in (27)–(28), we obtain the general sufficient condition for SLS:

If there exists a nonsingular matrix P such that for all times t

$$\begin{aligned} A^T(\Gamma(t), t)\,P + PA(\Gamma(t), t) &= -\alpha(\Gamma(t), t)\,P \\ A(\Gamma(t), t)\,P + PA^T(\Gamma(t), t) &= -\alpha(\Gamma(t), t)\,P \end{aligned} \tag{29}$$

then there is an SLS with respect to $-\bar{\alpha}/2$.

Particularly, if $P = J$, the relations (29) turn into

$$A^T(\Gamma(t), t)\,J + JA(\Gamma(t), t) = -\alpha(\Gamma(t), t)\,J \tag{30}$$

For $\alpha = \text{const}$, (30) is the sufficient condition obtained in ref. 4.

Although we have two matrix equations on the local stability matrix in the condition (29), some arguments exist[2] that the global stability matrix should have the same eigenvalues as the evolution matrix raised to the power of $1/t$ when $t \to \infty$ under some restrictions plausible for systems with a realistic interparticle interaction. In that case any equation of (29) (we will use the first one) can serve as a sufficient condition for an SLS.

We note that if P satisfies (29), then so does P^T and consequently the symmetric matrix $P + P^T$ and the antisymmetric matrix $P - P^T$, and at least one of which would be nondegenerate. Therefore we can search for only symmetric or antisymmetric matrices P satisfying condition (29) for our A. Since most physical systems are obtained by a modification of Hamiltonian systems for which P is antisymmetric, it is natural to look for only antisymmetric matrices P.

We now derive another sufficient condition for an SLS that may be more convenient for practical use. Consider a system whose equations of motion can be obtained from the ones of another system with an SLS (e.g., Hamiltonian) by an invertible time-independent linear phase-space transformation Q:

$$\Gamma' = Q^{-1}\Gamma \tag{31}$$

The local stability matrix corresponding to the new variables is then

$$A' = Q^{-1}AQ \tag{32}$$

The matrices A and A' are similar and according to the definitions (9) and (6) the corresponding evolution matrices are also similar. Though this similarity cannot be extended straightforwardly to the global stability matrices, if the conditions under which the latter has the same eigenvalues as the evolution matrix[2] are met, we can use (31) as a good sufficient condition for an SLS.

Suppose that for the old system the matrix P satisfying the first condition in (29) exists; then the new system also has such a matrix:

$$P' = Q^T P Q \tag{33}$$

As an example we consider the SLLOD equations[13] designed for the simulation of planar Couette flow in two dimensions, where N particles are subject to a constant shear rate $\gamma = \partial u/\partial y$, with u the mean flow velocity whose direction is chosen as the x axis. The equations of motion are

$$\begin{aligned} \dot{\mathbf{q}}_i &= \tilde{\mathbf{p}}_i/m + \mathbf{i}\gamma q_{iy} \\ \dot{\tilde{\mathbf{p}}}_i &= \mathbf{F}_i - \mathbf{i}\gamma \tilde{p}_{iy} \end{aligned} \tag{34}$$

where $\tilde{\mathbf{p}}_i = \mathbf{p}_i - \mathbf{i}mu$ is the *peculiar* momentum[13] of the ith particle defined as the part of the normal momentum $\mathbf{p}_i$ relevant for heat motion.

Though this system is not Hamiltonian, it has an SLS with respect to zero[7] because it can be reduced to a Hamiltonian system by a time-independent linear transformation: $p_{ix} \to p_{ix} - m\gamma q_{iy}$. Using (33), we find the matrix P' for which the condition (27) is satisfied:

$$P' = \begin{pmatrix} 0 & m\gamma I & (1/m)\, I & 0 \\ -m\gamma I & 0 & 0 & (1/m)\, I \\ -(1/m)\, I & 0 & 0 & 0 \\ 0 & -(1/m)\, I & 0 & 0 \end{pmatrix} \tag{35}$$

where each block is $N \times N$, and the phase space variables are in the following order: $q_{1x},..., q_{Nx}, q_{1y},..., q_{Ny}, p_{1x},..., p_{Nx}, p_{1y},..., p_{Ny}$ (the first index enumerates the particle, while the second one indicates the coordinate axis x or y).

4. SLS IN THERMOSTATTED SYSTEMS

Recently[7,8] an SLS property was discovered in dynamical systems serving as algorithms for nonequilibrium molecular dynamics simulations of fluids.[13] In these systems particles interact with each other via a Lennard-Jones-like potential and are also subject to an external force field. The existence of a steady state is guaranteed by the introduction of a thermostat removing the heat generated by the mechanical work done by this force.

The functional form of the thermostatted equations of motion is obtained from Gauss' principle of least constraint, stating that the actual motion in a system subject to constraints is the one that deviates minimally from the unconstrained motion. Gauss' principle is one of the equivalent variational principles introduced in the mechanics of nonholonomic systems (those with nonintegrable constraints).[14] The domain of applicability of all of them is strictly speaking unknown, but they were successfully applied to various practical problems.[15] The thermostatting procedure results in an additional viscous friction type force being exerted upon each particle. Although the procedure does not resemble the experimental situation, where the temperature is kept constant via the system boundaries, numerical simulations[7-9] so far show that it leads to results consistent with experimental data at least if the number of particles is sufficiently large. Use of the SLS property dramatically simplifies the procedure of calculating the transport coefficients of the system via LE[5,6] from using the sum of all of them to that of only two LE, e.g., the maximum and the minimum ones.[7]

First we show how to obtain equations of motion for thermostatted systems. Let the adiabatic (pertaining to a system of N particles without a thermostat), equations of motion in peculiar variables be of the form

$$\begin{aligned} \dot{\mathbf{q}}_i &= \mathbf{f}_i(\mathbf{q}, \tilde{\mathbf{p}}) \\ \dot{\tilde{\mathbf{p}}}_i &= \mathbf{g}_i(\mathbf{q}, \tilde{\mathbf{p}}) \end{aligned} \tag{36}$$

where Eqs. (36) may implicitly contain a heat-generating external field. Indices in this and the following sections range from 1 to N unless otherwise specified.

If the system is subject to the constraint

$$T(\mathbf{q}, \tilde{\mathbf{p}}, t) = \text{const} \tag{37}$$

then the actual value of $\dot{\tilde{\mathbf{p}}}_i$ corresponds to the minimum of the variable

$$C = \frac{1}{2} \sum_i \frac{1}{m_i} (\dot{\tilde{\mathbf{p}}}_i - \mathbf{g}_i)^2 \tag{38}$$

where m_i is the mass of the ith particle.

One can reformulate (37)–(38) as the requirement for the least possible effect of the constraint force upon the system.[14]

Expressing the constraint equation (37) in a $\dot{\tilde{\mathbf{p}}}_i$-dependent form, we have

$$\frac{dT}{dt} = \frac{\partial T}{\partial t} + \sum_i \left(\frac{\partial T}{\partial \mathbf{q}_i} \mathbf{f}_i + \frac{\partial T}{\partial \tilde{\mathbf{p}}_i} \dot{\tilde{\mathbf{p}}}_i \right) = 0 \tag{39}$$

Using the Lagrangian multiplier α, we obtain a convenient form of (37)–(38):

$$\frac{\partial}{\partial \dot{\tilde{\mathbf{p}}}_i}\left(C+\alpha\frac{dT}{dt}\right)=0 \tag{40}$$

It follows from (38)–(40) that the second equation in (36) can be replaced by

$$\dot{\tilde{\mathbf{p}}}_i=\mathbf{g}_i(\mathbf{q},\tilde{\mathbf{p}})-m_i\alpha\frac{\partial T}{\partial \tilde{\mathbf{p}}_i} \tag{41}$$

without any additional constraints. The functional form of $\alpha(\mathbf{q}, \tilde{\mathbf{p}}, t)$ is obtained by substituting (41) into (39), which yields

$$\alpha=\left\{\frac{\partial T}{\partial t}+\sum_i\left[\frac{\partial T}{\partial \mathbf{q}_i}\mathbf{f}_i+\frac{\partial T}{\partial \tilde{\mathbf{p}}_i}\mathbf{g}_i\right]\right\}\Big/\sum_i m_i\left(\frac{\partial T}{\partial \tilde{\mathbf{p}}_i}\right)^2 \tag{42}$$

This approach can be generalized to include any number of constraints.

We now show that if one disregards terms $O(1/N)$, and the adiabatic system is Hamiltonian and meets some generic requirements, then for the thermostatted system with the two types of constraints introduced below there is an SLS with respect to $-\bar{\alpha}/2$.

First consider the isokinetic constraint

$$T_{\text{kin}}=\sum\frac{\tilde{\mathbf{p}}_i^2}{2m_i}=\text{const} \tag{43}$$

Substituting (43) into (41) and (42), we obtain the equation for $\dot{\tilde{\mathbf{p}}}_i$:

$$\dot{\tilde{\mathbf{p}}}_i=\mathbf{g}_i(\mathbf{q},\tilde{\mathbf{p}})-\alpha\tilde{\mathbf{p}}_i \tag{44}$$

and the corresponding expression for α:

$$\alpha_{\text{kin}}=\frac{\sum_i(\tilde{\mathbf{p}}_i\mathbf{g}_i/m_i)}{\sum_i(\tilde{\mathbf{p}}_i^2/m_i)} \tag{45}$$

Due to anticipated mixing, we expect the interparticle forces and the momenta of the particles to be of the same order of magnitude, respectively, for sufficiently large times. Constructing then the local stability matrix A^{th}, we estimate the ratio of α to $\tilde{p}_i\,\partial\alpha/\partial\tilde{p}_j$ to be of order N, and the ratios of $\partial g_i/\partial q_j$ to $\tilde{p}_k\,\partial\alpha/\partial q_m$ also of order N if we assume in addition that the particle masses are all of the same order of magnitude and that the particles interact via a short-range potential (e.g., Lennard-Jones potential), i.e., that each particle effectively interacts with only $O(1)$ number of particles. Then in the limit of $N \to \infty$ we can neglect all the terms containing partial derivatives of α and in this approximation the matrix A^{th} has the form[7]

$$A^{\text{th}} = A^{\text{Ham}} - \frac{\alpha}{2}\begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix} - \frac{\alpha}{2}\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \tag{46}$$

The matrix A^{th} satisfies the sufficient condition (30) because the first two terms in (46) are infinitesimally symplectic matrices which satisfy (10).[7] Therefore the thermostatted system has an SLS with respect to $-\bar{\alpha}/2$.

If, on the other hand, the full internal energy is kept constant,

$$T_{\text{en}} = \sum_i \frac{\tilde{\mathbf{p}}_i^2}{2m_i} + \Phi(\mathbf{q}) = \text{const} \tag{47}$$

[where $\Phi(\mathbf{q})$ and $\mathbf{F}_i = -\partial\Phi/\partial\mathbf{q}_i$ are, respectively, the total potential energy and the force on the ith particle due to the other particles], then we still have Eq. (44), but with a different α:

$$\alpha_{\text{en}} = \alpha_{\text{kin}} - \frac{\sum_i \mathbf{F}_i \mathbf{f}_i}{\sum_i (\tilde{\mathbf{p}}_i^2/m_i)} \tag{48}$$

Although extra terms stemming from partial derivatives of α appear in this case in the local stability matrix, we are able to disregard them as well under the same assumptions as in the previous case.

Thus for both constraints in the limit of $N \to \infty$ the terms in the local stability matrix containing partial derivatives of α can be generically discarded. The local stability matrix for the thermostatted system is then of the form (46) and the SLS property follows from the SLS in the adiabatic system.

The question of whether the SLS property holds to all orders of $1/N$ terms is not resolved, but numerical simulations[7,9] suggest that it does. Supposing that for the adiabatic system (36) the sum of all Lyapunov exponents is zero and using (19), we can calculate the sum of all LE for the thermostatted system:

$$\sum_{k=1}^{2n} \lambda_i = \overline{\operatorname{tr} A} = -\overline{\sum_{k=1}^{n} \frac{\partial(\alpha \tilde{p}_k)}{\partial \tilde{p}_k}} = -\bar{\alpha}(n-2) - \bar{\beta} \tag{49}$$

Using (45) and (48), we obtain expressions for β for the two constraints, respectively:

$$\beta_{\text{kin}} = \alpha_{\text{kin}} + \left(\sum_{i,k=1}^{n} \frac{\tilde{p}_i \tilde{p}_k}{m_i} \frac{\partial g_i}{\partial \tilde{p}_k} \right) \Big/ \sum_{i=1}^{n} \frac{\tilde{p}_i^2}{m_i} \tag{50}$$

$$\beta_{\text{en}} = \beta_{\text{kin}} - \left(\sum_{i,k=1}^{n} F_i \tilde{p}_k \frac{\partial f_i}{\partial \tilde{p}_k} \right) \Big/ \sum_{i=1}^{n} \frac{\tilde{p}_i^2}{m_i} \tag{51}$$

Thus if an SLS holds with the $1/N$ terms being taken into account, we see from (49) that the symmetry constant will also have $1/N$ corrections, since it is given by $-\frac{1}{2}[\bar{\alpha}(1-2/n)-(1/n)\bar{\beta}]$ instead of $-\bar{\alpha}/2$.

5. SLS IN COLOR CONDUCTIVITY

As a typical example we consider the color conductivity algorithm,[16] designed for the study of self-diffusion of identical particles, which we generalize here by adding a "magnetic" field. Consider a two-dimensional system of two kinds of particles, each having the same mass m but different color "charge" $c_i = \pm 1$. The entire system is color neutral. All particles are subject to a constant external color field F_c applied along the x direction and to a constant external "magnetic" field B applied along the z direction. The adiabatic equations of motion in normal (nonpeculiar) variables and in two dimensions can be derived from the Hamiltonian

$$H_{\text{col}} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \Phi(\mathbf{q}) - F_c \sum_i c_i q_{ix} + B \sum_i c_i [q_{ix} p_{iy} - q_{iy} p_{ix}] \tag{52}$$

The color field generates a current per particle along the x direction:

$$J_x = \frac{1}{N} \sum_i \frac{c_i p_{ix}}{m} \tag{53}$$

but does not affect the mean velocity in the y direction:

$$J_y = \frac{1}{N} \sum_i \frac{p_{iy}}{m} \tag{54}$$

It is natural to require for the peculiar momenta $\sum_i c_i \tilde{p}_{ix} = 0$, as there should be no peculiar current[13] and $\sum_i \tilde{p}_{iy} = 0$, as the mean peculiar velocity in the y direction should be equal to zero as well. Thus, we define peculiar momenta in this case as follows:

$$\begin{aligned} \tilde{p}_{ix} &= p_{ix} - mc_i J_x \\ \tilde{p}_{iy} &= p_{iy} - mJ_y \end{aligned} \tag{55}$$

The transformation (55) is degenerate due to the linear dependence of the peculiar momenta.

We rewrite the adiabatic equations of motion in peculiar variables and apply Gauss' principle with the isokinetic constraint to obtain

$$\begin{aligned}
\dot{q}_{ix} &= \frac{\tilde{p}_{ix}}{m} - c_i B q_{iy} + c_i J_x(t) \\
\dot{q}_{iy} &= \frac{\tilde{p}_{iy}}{m} + c_i B q_{ix} + J_y(t) \\
\dot{\tilde{p}}_{ix} &= F_{ix} - \frac{c_i}{N} \sum_k c_k F_{kx} - c_i B \tilde{p}_{iy} - \alpha \tilde{p}_{ix} \\
\dot{\tilde{p}}_{iy} &= F_{iy} + c_i B \tilde{p}_{ix} - \alpha \tilde{p}_{iy}
\end{aligned} \tag{56}$$

with $J_x(t)$ and $J_y(t)$ independent of the peculiar variables. From (45) we find the functional form of α for the Eqs. (56):

$$\alpha(\mathbf{q}, \tilde{\mathbf{p}}) = \frac{\sum_i \mathbf{F}_i \tilde{\mathbf{p}}_i}{\sum_i \tilde{\mathbf{p}}_i^2} \tag{57}$$

The procedure in ref. 16 where the equations of motion are written in terms of normal (nonpeculiar) variables yields the same expression (57) as well as the same local stability matrix up to terms of the order of $1/N$. In the absence of the "magnetic" field the expression for α is not affected by the choice of normal or peculiar y components of the momenta, because in this case we suppose that the mean velocity in Eq. (54) is already zero in normal variables in the stationary state. But if $B \neq 0$, the choice of normal y components of momenta would result in the dependence of α upon the "magnetic" field, which is unnatural, since the latter does not generate any heat to be removed. We also note that while the color field F_c is absent from the equations in peculiar variables, the "magnetic" field terms in the equations are not affected by the choice of normal or peculiar variables (55).

As in the previous section, the local stability matrix for the Eqs. (56) is of the form (46) in the limit of $N \to \infty$ and therefore the system has an SLS with respect to $-\bar{\alpha}/2$ as an asymptotic property. As for the $1/N$ corrections to the symmetry constant, from (50) and (51) we find that for the color conductivity equations (56) $\beta_{\text{kin}} = \alpha_{\text{kin}}$ and $\beta_{\text{en}} = 0$. Thus for this system with or without "magnetic" field the sum of all Lyapunov exponents is proportional to $\bar{\alpha}$ with an N-dependent coefficient regardless of whether the constraint is isokinetic or isoenergetic. This is not true for Hamiltonian systems in general. In fact, for the thermostatted DOLLS equations[13] which can simulate planar Couette flow in the linear regime[13] $\beta_{\rm en} = -(\gamma \sum_i \tilde{p}_{ix} \tilde{p}_{iy})/(\sum_i \tilde{\mathbf{p}}_i^2)$ and $\beta_{\rm kin} = \alpha_{\rm kin} + \beta_{\rm en}$. The last relationship is also not universal for Hamiltonian systems: it is specific to Hamiltonians of the form

$$H = \frac{\tilde{\mathbf{p}}^2}{2m} + \Phi(\mathbf{q}) + \sum_{i,k=1}^{n} a_{ik} q_i \tilde{p}_k + \sum_{k=1}^{n} b_k \tilde{p}_k$$

where a_{ik} and b_k do not depend on the coordinates and momenta.

The SLS property for the color conductivity and the DOLLS equations was confirmed numerically in ref. 8. The Gaussian thermostats can also be applied to the SLLOD equations (34) and an SLS in the resulting system was also observed,[7,8] but to prove this analytically for all short-range potentials remains a challenge.

6. CONCLUSION

As we have demonstrated, even for the systems considered in this paper the question of Lyapunov spectrum symmetry remains open. While the Eqs. (56) suggest for a system with a finite number of particles N at best a symmetry with respect to an N-dependent constant, this symmetry has so far been proved only neglecting the $1/N$ terms. There is also the problem of the evaluation of the symmetry constant for finite N.

It should be pointed out, though, that insofar as the Lyapunov exponents are connected to the transport coefficients [cf. Eq. (11) of ref. 7] a very large (effectively infinite) number of particles is involved, since the transport coefficients are defined in that limit.

We remark that we did not take into account the first integrals of the system and the zero LE associated with them in the treatment of an SLS, so the question of the existence of an SLS in that case remains open.

It would be extremely useful to establish a connection between the SLS property and other easily verified symmetries of the system. Conservation of phase volume in the adiabatic case was shown[8] to be insufficient for an SLS. This is not surprising since this symmetry requires only the sum of all local eigenvalues to be zero; then according to (19) the sum of *all* LE is also zero, but this bears no relation to SLS (which implies that the sums of each conjugate pair of Lyapunov exponents are equal), as was demonstrated on an example in ref. 12. Time-reversal invariance (TRI) is not necesary for SLS either, the simplest counterexample being a Hamiltonian system with a Hamiltonian linear in the momenta.[17] Such a system has SLS, but does not have TRI. Some questions related to TRI and SLS are investigated in ref. 18.

ACKNOWLEDGMENTS

The authors are grateful to Prof. M. J. Feigenbaum for fruitful discussions. A.S.K. and E.G.D.C. also acknowledge financial support from the Department of Energy under Contract No. DE-FG02-88-ER13847.

REFERENCES

1. G. Benettin, L. Galgani, A. Giorgilli, and J. M. Strelcyn, *Meccanica* **15**:9 (1980).
2. I. Goldhirsch, P. L. Sulem, and S. A. Orszag, *Physica D* **27**:311 (1987).
3. V. I. Arnold, *Mathematical Methods in Classical Mechanics* (Springer-Verlag, Berlin, 1978).
4. U. Dressler, *Phys. Rev. A* **38**:2103 (1988).
5. W. G. Hoover and H. A. Posch, *Phys. Lett. A* **123**:227 (1987).
6. H. A. Posch and W. G. Hoover, *Phys. Rev. A* **39**:2175 (1989).
7. D. J. Evans, E. G. D. Cohen, and G. P. Morris, *Phys. Rev. A* **42**:5990 (1990).
8. S. Sarman, D. J. Evans, and G. P. Morris, *Phys. Rev. A* **45**:2233 (1992).
9. G. P. Morris, *Phys. Rev. A* **37**:2118 (1988).
10. J. P. Eckman and D. Ruelle, *Rev. Mod. Phys.* **57**:617 (1985).
11. W.-H. Steeb and A. Kunick, *Phys. Rev. A* **25**:2889 (1982).
12. D. Gupalo, in *NEEDS'92 Proceedings*, V. G. Makhankov and O. K. Pashaev, eds. (World Scientific, Singapore, 1993).
13. D. J. Evans and G. P. Morriss, *Statistical Mechanics of NonEquilibrium Liquids* (Academic Press, London, 1990).
14. L. A. Pars, *A Treatise on Analytical Dynamics* (Oxbow Press, Woodbridge, Connecticut, 1979).
15. Ju. I. Naimark and N. A. Fufaev, *Dynamics of Nonholonomic Systems* (AMS, Providence, Rhode Island, 1972).
16. A. Baranyai, D. J. Evans, and E. G. D. Cohen, *J. Stat. Phys.* **70**:1085 (1993).
17. J. A. G. Roberts and G. R. W. Quispel, *Phys. Rep.* **216**:63 (1992).
18. A. S. Kaganovich and D. Gupalo, Time-reversibility, ergodicity and Lyapunov exponents in thermostatted systems, preprint, Rockefeller University (1993).