Journal of Statistical Physics, Vol. 86, Nos. 5/6, 1997

Applications of Periodic Orbit Theory to *N*-Particle Systems

Lamberto Rondoni[1,2] **and Gary P. Morriss**[1]

Received July 6, 1996; final September 10, 1996

In recent years a number of new techniques have become available in nonequilibrium statistical mechanics, all derived from dynamical system theory, especially from the thermodynamic formalism of Ruelle. We focus here on periodic orbit theory, and we compare it with a novel approach proposed by Evans, Cohen, and Morriss, and developed further by Gallavotti and Cohen. We argue that the two approaches based on such theories are equivalent for systems of many particles if the underlying dynamics is similar to that of Anosov systems, and that such equivalence should remain in more general situations. We extend our previous explanation of irreversibility in the thermostatted Lorentz gas to *N*-particle diffusion and shearing systems.

KEY WORDS: Gaussian thermostat; orbital measures; Ruelle's principle; stability eigenvalues.

1. INTRODUCTION

It has been recently noted that the language of dynamical system theory constitutes a unifying framework for both equilibrium and nonequilibrium statistical mechanics.[1,2] In fact, both can be studied from the viewpoint of the dynamics associated with a given differential equation or mapping. In particular, many works have appeared in the nonequilibrium statistical mechanics literature which in one way or another make use of ideas from dynamical systems theory, producing many important results. For further information, we refer the reader to refs. 3–12, which represent just a small fraction of the available literature, and to ref. 13, which presents a thoughtful synthesis of some of the most important results in the field. Also, there

[1] School of Physics, University of New South Wales, Sydney 2052, Australia.
[2] Permanent address: Dipartimento di Matematica, Politecnico di Torino, I-10129 Turin, Italy.

0022-4715/97/0300-0991$12.50/0

have been attempts to build a consistent theory of nonequilibrium systems with the tools of the thermodynamic formalism of Ruelle. Most notable among these are the recent works by Dorfman and Gaspard on the escape rate formalism for open systems.[14] However, it is in ref. 1 that the need to justify these ideas on the grounds of a new fundamental principle has been pointed out and a candidate for such a principle has been introduced.

Given the importance and relevance for our own work of the arguments presented in ref. 1, we summarize them as follows. Because the numerical simulations of ref. 15 for shearing flows show a strong correlation between purely dynamic and thermodynamic quantities, the authors argue that this is due to an underlying general structure derivable from a fundamental principle. More precisely, they attempt to identify a counterpart in nonequilibrium statistical mechanics for the microcanonical ensemble of equilibrium statistical mechanics, and they propose that Ruelle's principle (**R**)—introduced in ref. 16—be invoked for this purpose. Quoting from ref. 1, principle **R** states that "the time averages of observables, on motions with initial data randomly sampled with the Liouville distribution $\bar{\mu}_0$, are described by a stationary probability distribution $\bar{\mu}$ obtained by attributing a suitable probability density to the surface elements of the unstable manifolds of the points in phase space." This amounts to saying that a new type of ensemble is to be used in nonequilibrium problems, which reduces to the usual microcanonical ensemble at equilibrium (in agreement with what is found, for instance, in refs. 2, 11, 17, and 18 for the Lorentz gas) and that coincides with the Sinai–Ruelle–Bowen (SRB) measure for smooth hyperbolic dynamical systems. The only nonequilibrium system of particles where the validity of **R** has been rigorously proven is the nonequilibrium Lorentz gas at small external fields,[19] for which numerical investigations in terms of periodic orbits[11] are now available.

Gallavotti and Cohen focus on related many-particle models, and in particular they develop the idea proposed in ref. 15 of deriving the stationary measure of a shearing system from a limiting process involving trajectory segments in phase space. Then they argue that the validity of **R** for such systems rests on a "chaotic hypothesis," which in their formulation says that "...the many particle systems in statistical mechanics are essentially chaotic in the sense of Anosov, i.e., they behave *as if they were* Anosov systems as far as their properties of physical interest are concerned." Moreover, they point out that such a hypothesis should hold at least in the thermodynamic limit. Gallavotti and Cohen then proceed to consider dissipative, time-reversible, transitive Anosov systems, and their analysis leads to, among other things, the conclusion that the use of Eq. (6.3) in ref. 1 is justified for such systems (see ref. 20 for related rigorous

results and proofs). In this way, the measure they propose is shown to have a meaning for a large class of dynamical systems, as does the measure based on periodic orbits of Axiom A systems, which has been known and used for long time.[21,22] The apparent reduced generality of the method of ref. 1 as opposed to the periodic orbit aproach, does not concern us, as our focus is on time-reversible systems, and we are not aware of a reversible Axiom A system which is not also Anosov.[23] That any system of particles obeys the chaoticity assumption in the form given by Gallavotti and Cohen is not known at present, so it is not known that principle **R** actually holds for systems other than Axiom A systems and those of ref. 19. However, the numerical test provided by ref. 15, as well as the indirect tests provided by the other works mentioned above, do make a strong case in favor of the validity of **R**, either as stated by Gallavotti and Cohen or in some related form.

The popular technique of periodic orbit theory has been successfully applied to practical calculations of the properties of many low-dimensional, hyperbolic dynamical systems.[24] Among the many interesting features of this approach, we find that[25] (a) orbits are hierarchically ordered (short cycles give good approximations to a nonwandering set); and (b) orbit stability eigenvalues are structurally robust (they change smoothly with parameter changes).

Point (b), in particular, is important for the unification of equilibrium and nonequilibrium systems in a single framework. For instance, it was noticed in ref. 11 that orbits of finite length and their stability properties change smoothly over wide ranges of the applied external field, starting from the equilibrium zero-field case. Nonetheless, the computational difficulty in finding all the periodic orbits of systems with an arbitrary number of dimensions has so far prohibited the application of periodic orbit theory to more general N-particles systems. For instance, the nonequilibrium systems in refs. 11, 26, and 27 all deal with one- or two-particle systems. These studies aim at showing that periodic orbit expansions can be applied to systems other than Axiom A (or Anosov), as indeed the nonequilibrium Lorentz gas is not a smooth dynamical system, and that they can be applied outside the linear regime of ref. 19, since they yield good results for rather large fields, at least where hyperbolicity and ergodicity still seem to hold.

In this work we intend to go one step further in the application of periodic orbit theory and show that it can be used with profit in the study of many-particle systems. In such a context the periodic orbit method can then be regarded as largely equivalent to the technique of ref. 1. In fact, despite the lack of a proof of the validity of either of the two approaches, the underlying mathematical structure seems to be the same (Anosov-like),

and we expect that if one of the two methods works, the other also does. Assuming this to be the case, we have a trivial example of "equivalence of ensembles" in nonequilibrium statistical mechanics, trivial because the stationary ensembles derived with the method of ref. 1 and from periodic orbits ought to be the same SRB measure. Moreover, as pointed out by a referee, this equivalence is already known in the mathematical literature on Axiom A systems (see e.g., Chapter 7 of ref. 21). If this is shown to hold for wider classes of dynamics (perhaps in some sort of thermodynamic limit), it may result in a very important understanding of the physics of nonequilibrium systems, and it would justify the use of the most convenient paradigm among those that are available. As a matter of fact, there are speculations that this might be the case,[16] based on the expected equivalence of stationary distributions produced by dynamics with stochastic[28] and Gaussian[29] thermostats, which are respectively absolutely continuous and singular with respect to the Liouville measure. Other arguments in favor of an equivalence of ensembles for nonequilibrium systems can be found in ref. 39.

Throughout this paper we assume that some form of the chaoticity hypothesis of Gallavotti and Cohen is satisfied by the dynamics of our systems of particles, so that they behave as if they were Anosov. This in turn justifies our use of periodic orbit theory, as it implies that unstable periodic orbits are dense in the relevant attractor and that the weak limit of weighted orbital measures in the limit of large period is the corresponding SRB measure. This work is organized as follows. In Section 2 we introduce our notation and produce preliminary results for the case of many particles subjected to a constant external field and a Gaussian thermostat. Section 3 repeats the same for the problem of refs. 1 and 15, i.e., many-particle, thermostatted shearing flow. Section 4 shows some examples of how these results may be used in periodic orbit theory. Section 5 concludes this work with general comments.

2. THE CASE OF A CONSTANT EXTERNAL FIELD

In this section we consider a system of N spherical particles (so that rotational degrees of freedom can be ignored) which are subject to a constant external field. The interactions among the particles can be hard core or soft core, as long as they derive from a scalar potential. We also assume that there is a Gaussian thermostat[29] which fixes either the kinetic or the internal energy (depending upon the choice of ensemble), and that the system is periodic, so that there is a fundamental domain whose replicas tile the whole phase space. In the case of hard-core interactions the particles feel the effect of the external field, but do not influence each other at

large distance. Their charge is called a "color charge" and the external field is called a "color field." The case of long-range interactions, instead, concerns electrically charged particles in an external field of force. The reader should note that the resulting equations of motion are not Hamiltonian, and thus they cannot be derived from quantum mechanics in the limit of vanishing h. As a consequence, the introduction of the fluctuating, deterministic, frictionlike force due to the thermostat may initially seem unphysical. However, it has been used extensively to treat many-particle systems in the computer simulation of thermal transport properties[5] and its theoretical standing there is firm. It has been shown that this thermostatting mechanism is optimal[6] in the sense that it obeys Gauss' principle of least constraint and that it preserves the reversibility of the equations of motion. Also, the value of the transport coefficient is directly related to the average thermostatting multiplier[7] and there is numerical evidence for a direct relation between the transport coefficient and the sum of conjugate pairs of Lyapunov exponents.[3,8,30] But by far the most important effect of the thermostat is that it guarantees the existence of a stationary state for a large range of values of the field, and therefore the existence of an attractor.

Consider a system of N particles in d dimensions, with no restrictions on the mass m_i and the charge c_i of each one of them. Since the thermostat removes one degree of freedom and conservation of momentum removes d degrees of freedom, a kinetic temperature can be defined by

$$kT = \frac{1}{dN - d - 1} \sum_{i=1}^{N} \frac{1}{m_i} (\mathbf{p}_i - \mathbf{p}_0)^2 \tag{1}$$

where the velocity of the center of mass, $\mathbf{p}_0 = m\dot{\mathbf{q}}_0$, say, is subtracted from the individual velocities to obtain the thermal momenta $(\mathbf{p}_i - \mathbf{p}_0)$, and the denominator is simply the number of degrees of freedom of the system. In all that follows we keep close account of both order-N and order-one terms. No approximations are made. The equations of motion for this system are

$$\dot{\mathbf{q}}_i = \frac{\mathbf{p}_i}{m}; \qquad \dot{\mathbf{p}}_i = \mathbf{F}_i + c_i \mathbf{F}_e - \alpha \mathbf{p}_i \tag{2}$$

where $\mathbf{F}_i$ is the total force exerted on particle i by all of the other particles, $\mathbf{F}_e$ is the constant external field, and α is obtained from Eqs. (2) by imposing the constraint that the kinetic energy of the system K is a constant of motion. Thus α takes the form

$$\alpha = \frac{1}{2K} \left(\mathbf{J} \cdot \mathbf{F}_e + \sum_{i=1}^{N} \frac{1}{m_i} \mathbf{p}_i \cdot \mathbf{F}_i \right) \tag{3}$$

where the current $\mathbf{J}$ is defined by

$$\mathbf{J} = \sum_{i=1}^{N} c_i \dot{\mathbf{q}}_i = \sum_{i=1}^{N} \frac{c_i}{m_i} \mathbf{p}_i \tag{4}$$

Many of the results that are presented here arise from the behavior of the stability eigenvalues (also called Lyapunov numbers) to variations in the external field. The stability eigenvalues are determined from the eigenvalues of the linearized time evolution operator $\mathsf{L}(t)$. This operator gives the time evolution of the set of infinitesimal tangent vectors for the dynamical system and is related[8] to the local stability matrix T by

$$\begin{aligned} \mathsf{L}(t) &= \exp_L \int_0^t ds\, \mathsf{T}(\mathbf{\Gamma}(s)) \\ &= \mathsf{I} + \sum_{n=1}^{\infty} \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n\, \mathsf{T}(s_1)\, \mathsf{T}(s_2) \cdots \mathsf{T}(s_n) \end{aligned} \tag{5}$$

where I is the identity matrix, $\mathit{\Gamma}(s) = (\mathbf{q}_1(s), \mathbf{p}_1(s), \ldots, \mathbf{p}_N(s))$ is the phase point at time s, while the stability matrix for smooth dynamics (along free flights, for example) is given by $\mathsf{T} = \partial \dot{\mathbf{\Gamma}} / \partial \mathbf{\Gamma}$. The symbol $\exp_L \int_0^t \mathsf{T}(s)\, ds$ is usually called a left-ordered exponential or time-ordered integral. It can be obtained as a product of infinitesimal time evolution operators whose exponents do not necessarily commute with each other. If the commutator $[\mathsf{T}(u), \mathsf{T}(v)] = 0$ for all times $u, v \in [0, t]$, then the left-ordered exponential reduces to the normal exponential of the integral of T, whose eigenvalues are the exponentials of the eigenvalues of the integral of T. If the dynamics is not smooth, as in the case of hard-core particles, the evolution operator $\mathsf{L}(t)$ can be expressed as an ordered product of free-flight and collision terms. The stability eigenvalues for the corresponding dynamical system are the eigenvalues of the symmetric matrix $\mathit{\Lambda}$, where[31]

$$\mathit{\Lambda} = \lim_{t \to \infty} \mathit{\Lambda}(t) = \lim_{t \to \infty} (\mathsf{L}(t)^T \cdot \mathsf{L}(t))^{1/2t}$$

For almost all initial conditions the stability eigenvalues of the system are only defined in the limit as $t \to \infty$. However, for an initial condition which corresponds to a periodic orbit, we need only consider $\mathit{\Lambda}(t)$ for one traversal of the orbit, because subsequent traversals simply reproduce the same pattern. Obviously, the computation of all the stability eigenvalues for each orbit of a many-particle system is a task beyond our present ability. However, in the approach based on periodic orbits the single stability eigenvalues are not needed; generally the product of the expanding ones is

enough; moreover, in the qualitative analysis we perform in Section 4 the determinant of the stability matrix suffices.

Before constructing the stability matrix for color diffusion we need to define the notation that will be used throughout this paper. First we observe that a system of N particles is mechanically equivalent to a system of $n = N - 1$ particles. The redundant variables may be eliminated using the conserved quantities, the center-of-mass position, and the total momentum. Alternatively a coordinate transformation from $(\mathbf{q}_1, \ldots, \mathbf{q}_{N-1}, \mathbf{q}_N)$ to $(\mathbf{q}_1, \ldots, \mathbf{q}_{N-1}, \mathbf{q}_0)$, where $\mathbf{q}_0$ is the position of the center-of-mass, and a similar transformation for the momenta is sufficient. The equations of motion for $\mathbf{q}_0$ and $\mathbf{p}_0$ are trivial and can be removed from the stability matrix. Of the remaining $2dn$ variables (in d dimensions), all but one of the variables are independent, the other being determined by the constraint of constant kinetic energy (or constant kinetic temperature). For ease of notation we will construct a $2dn \times 2dn$ stability matrix. Note that in calculating the effect of an arbitrary variation due to a change in a single variable, the kinetic energy itself may vary. Treating the kinetic energy as a phase variable and using the equation for α takes explicit account of the constant kinetic energy constraint in the $2dn \times 2dn$ stability matrix.

For a two-dimensional coordinate space the stability matrix T is made up of four $2n \times 2n$ blocks, and it can be represented by

$$\mathsf{T} = \begin{pmatrix} \dfrac{\partial}{\partial \mathbf{q}_i} \dot{\mathbf{q}}_j & \dfrac{\partial}{\partial \mathbf{p}_i} \dot{\mathbf{q}}_j \\ \dfrac{\partial}{\partial \mathbf{q}_i} \dot{\mathbf{p}}_j & \dfrac{\partial}{\partial \mathbf{p}_i} \dot{\mathbf{p}}_j \end{pmatrix}$$

where we give the form of the ijth subblock of each of the $2n \times 2n$ blocks. For color diffusion these subblocks are given by

$$\frac{\partial}{\partial \mathbf{q}_i} \dot{\mathbf{q}}_j = 0, \qquad \frac{\partial}{\partial \mathbf{p}_i} \dot{\mathbf{q}}_j = \frac{1}{m_i} \delta_{ij}^{\mu\nu}$$

$$\frac{\partial}{\partial \mathbf{q}_i} \dot{\mathbf{p}}_j = \Psi_{ij} - \frac{1}{2K} \sum_k \Psi_{ik} \cdot \mathbf{p}_k \mathbf{p}_j, \quad \frac{\partial}{\partial \mathbf{p}_i} \dot{\mathbf{p}}_j = -\delta_{ij}^{\mu\nu} \alpha - \frac{1}{2K} \left(\frac{1}{m_i} (\mathbf{F}_i + c_i \mathbf{F}_e) - 2\alpha \mathbf{p}_i \right) \mathbf{p}_j$$

The delta $\delta_{ij}^{\mu\nu}$ is equal to one if both $i = j$ and $\mu = \nu$, where $\mu, \nu \in \{x, y\}$. The matrix Ψ is composed of $d \times d$ blocks, where the ijth block is given by $\partial \mathbf{F}_j / \partial \mathbf{q}_i$.

For simplicity, consider the external field to be parallel to the x axis, so that $\mathbf{F}_e = (F_e, 0)$. We deal first with the isokinetic dynamics of hard

spheres, and note that collisions among any number of them occur at discrete times. In fact, as in ref. 1, the collision times may be used to identify a Poincaré section for the system. The equations of motion for a free flight are

$$\dot{x}_i = p_{ix}/m_i, \qquad \dot{y}_i = p_{iy}/m_i$$
$$\dot{p}_{ix} = c_i F_e - \alpha p_{ix} \qquad \dot{p}_{iy} = -\alpha p_{iy}$$

and the thermostatting multiplier reduces to

$$\alpha = \frac{F_e}{2K} \sum_{i=1}^{N} c_i \frac{p_{ix}}{m_i} \equiv \sum_{i=1}^{N} \varphi_i p_{ix} = \frac{F_e J_x}{2K}, \qquad \text{where} \quad \varphi_i = \frac{c_i F_e}{2m_i K}$$

Here $\mathbf{J} = (J_x, J_y)$ is the dissipative current associated with a given trajectory. The determinant of $\mathsf{L}(t) = \exp_L \int_0^t \mathsf{T}(s)\, ds$, limited to a free flight, is given by

$$\ln \det(\mathsf{L}(t)) = -(2n-1) \int_0^t \alpha(s)\, ds \tag{6}$$

If at time t some particles collide, the evolution operator for the tangent vectors from time zero up to immediately after the collision t^+ can be expressed as

$$\mathsf{L}(t) = \mathsf{L}_c(t)\, \mathsf{L}_f(t) = \mathsf{L}_c(t) \exp_L \int_0^t \mathsf{T}(s)\, ds$$

where $\mathsf{L}_c(t)$ is the collision operator at time t and $\mathsf{L}_f(t)$ is the corresponding free-flight contribution. Because hard-core collisions preserve the Liouville measure, we have that the determinant of $\mathsf{L}_c(t)$ is one. Thus, the determinant of the stability matrix relative to a given trajectory is simply the product of the determinants corresponding to the free flights, and this implies that relation (6) holds for a generic trajectory and for an arbitrary time t.

For a periodic orbit of period τ the internal energy

$$H_0(\mathbf{q}, \mathbf{p}) = \frac{1}{2} \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{m_i} + \frac{1}{2} \sum_{i,j=1}^{N} \phi_{ij}(q_{ij})$$

is also periodic; thus we can integrate over a complete period to write

$$(dn-1) \int_0^\tau ds\, \alpha(s) = \frac{1}{kT} \mathbf{F}_e \cdot \int_0^\tau ds\, \mathbf{J}(s) \tag{7}$$

from which we obtain the Lyapunov sum rule

$$-\sum_{i=1}^{2dn} \lambda_i = \frac{dn-1}{\tau} \int_0^\tau ds\, \alpha(s) = \frac{1}{\tau kT} \mathbf{F}_e \cdot \int_0^\tau ds\, \mathbf{J}(s) \tag{8}$$

which generalizes the sum rule for the nonequilibrium Lorentz gas[2,11,26] to the case of many hard spheres subject to a color field. Here, λ_i is the ith Lyapunov exponent of the given orbit.

The results for hard spheres can be readily generalized to the case of interactions which derive from a scalar potential. In fact, in two dimensions we have

$$\dot{x}_i = p_{ix}/m_i, \qquad \dot{y}_i = p_{iy}/m_i$$

$$\dot{p}_{ix} = F_{ix} + c_i f_e - \alpha p_{ix}, \qquad \dot{p}_{iy} = F_{iy} - \alpha p_{iy} \qquad \forall i$$

where $\mathbf{F}_i = (F_{ix}, F_{iy})$, the total force exerted on particle i by the remaining $N-1$ particles, is assumed to be a function of the relative positions of the particles only. Then, for T we have

$$\mathsf{T} = \begin{pmatrix} 0 & \mathbf{M} \\ \Psi' & \mathbf{A} \end{pmatrix} \qquad \text{with} \quad \Psi'_{ij} = \Psi_{ij} - \frac{1}{2K} \sum_k \Psi_{ik} \cdot \frac{1}{m_k} \mathbf{p}_k \mathbf{p}_j$$

where

$$\Psi_{ij} = \partial \mathbf{F}_i / \partial \mathbf{q}_j$$

The block $\mathbf{M}$ is the same as for the hard-core case, while the block $\mathbf{A}$ is modified by the fact that the thermostat α contains a collisional term depending on configurations:

$$\alpha = \sum_{i=1}^{N} \left[\frac{\mathbf{F}_i \cdot \mathbf{p}_i}{2m_i K} + \varphi_i p_{ix} \right] = -\frac{\dot{\Phi}}{2K} + \sum_{i=1}^{N} \varphi_i p_{ix}$$

where Φ is the total potential energy. Because Ψ' contributes no terms to the trace of the integral of T, the only modifications to Eq. (6) for the case of long-range interactions comes from the diagonal terms, and we get

$$\ln \det(\mathsf{L}(t)) = -(2n-1) \int_0^t \alpha(s)\, ds$$

$$= -(2n-1) \left\{ \Phi(\Gamma(t)) - \Phi(\Gamma(0)) + \sum_{i=1}^{N} m_i \varphi_i \Delta x_i(t) \right\}$$

Thus, with a minor change, the result for hard spheres under the effect of a color field can be extended to the case of electrically charged particles. In particular, for potentials depending on the inverse of the distance between particles, we note that their singularities could constitute a problem, although the work done by the interaction forces vanishes if we consider a periodic orbit (up to a lattice translation). Thus, for soft-sphere potentials, it is more natural to fix the total internal energy of the system rather than its kinetic energy. To fix this quantity in time, we must impose the condition that

$$\frac{dH_0}{dt} = 0$$

and since $\mathbf{F}_e$ has vanishing component along the y direction, we deduce that

$$\alpha = \frac{F_e}{2K} \sum_{i=1}^{N} \frac{c_i}{m_i} p_{ix} = \sum_{i=1}^{N} \varphi_i p_{ix} \tag{9}$$

which is the same expression we found for the isokinetic dynamics of hard spheres. This was to be expected, indeed, because in the hard-sphere case the total energy of the particles is purely kinetic. We conclude that Eq. (8) holds for all trajectories with soft interaction potentials, when the dynamics is isoenergetic.

3. THE SHEAR FLOW CASE

With the same techniques as used in Section 2 we now study a system of N particles subjected to shear. The SLLOD equations of motion are

$$\dot{\mathbf{q}}_i = \frac{1}{m_i} \mathbf{p}_i + \mathbf{n}_x \gamma y_i, \qquad \dot{\mathbf{p}}_i = \mathbf{F}_i - \mathbf{n}_x \gamma p_{yi} - \alpha \mathbf{p}_i$$

where

$$\alpha = \frac{\sum_{i=1}^{N} (\mathbf{F}_i \cdot \mathbf{p}_i - \gamma p_{xi} p_{yi})}{\sum_{i=1}^{N} \mathbf{p}_i^2}$$

It can be shown that the elements of the stability matrix are then

$$\frac{\partial}{\partial \mathbf{q}_i}\dot{\mathbf{q}}_j = \delta_{ij}^{yx}\gamma, \qquad \frac{\partial}{\partial \mathbf{p}_i}\dot{\mathbf{q}}_j = \frac{1}{m_i}\delta_{ij}^{\mu\nu}$$

$$\frac{\partial}{\partial \mathbf{q}_i}\dot{\mathbf{p}}_j = \Psi_{ij} - \frac{1}{\sum \mathbf{p}_m^2}\sum_k \Psi_{ik}\cdot \mathbf{p}_k \mathbf{p}_j$$

$$\frac{\partial}{\partial \mathbf{p}_i}\dot{\mathbf{p}}_j = -\delta_{ij}^{\mu\nu}\alpha - \delta_{ij}^{yx}\gamma - \frac{1}{\sum \mathbf{p}_m^2}(\mathbf{F}_i - \mathbf{n}_x \gamma p_{yi} - \mathbf{n}_x \gamma p_{yi} - 2\alpha \mathbf{p}_i)\,\mathbf{p}_j$$

where $\delta_{ij}^{yx} = 1$ for the term which corresponds to the y component of i and the x component of j, and zero otherwise.

First we consider a hard-core, isokinetic system, so that stability matrix only contains the free-flight components. These are

$$\dot{x}_i = p_{ix}/m_i + \gamma y_i, \qquad \dot{y}_k = p_{iy}/m_i$$

$$\dot{p}_{ix} = -\gamma p_{iy} - \alpha p_{ix}, \qquad \dot{p}_{iy} = -\alpha p_{iy}$$

where

$$\alpha = -\frac{\gamma}{2K}\sum_{i=1}^{N}\frac{1}{m_i}p_{ix}p_{iy}$$

Therefore, the logarithm of the determinant of the evolution operator for tangent vectors $\mathsf{L}(t)$ is given by

$$\ln \det(\mathsf{L}(t)) = \mathrm{Tr}\int_0^t \mathsf{T}(s)\,ds = -2n\int_0^t ds\,\alpha(s) \tag{10}$$

Note that the time average of α over a generic chaotic trajectory is related to the average shear stress for the system (which we assume to be ergodic). This equation is consistent with the Lyapunov sum rule for shear flow obtained previously.[3]

If the interactions among the spheres are soft and derive from a scalar potential, the null block in the definition of T for hard spheres is replaced by a block Ψ which is identical to the one for the case of constant color field. This block does not contribute to the trace of T; however, its presence changes the form of the thermostat α, so that the determinant of $\mathsf{L}(t)$ for isokinetic dynamics has other terms besides those relative to the pressure tensor. As in the case of constant external field, these extra terms are related to the work done by the interaction forces. Thus, if we fix the total energy for our shearing flow, we find that the thermostat α takes the same

form as for the isokinetic, hard-sphere case, and that the determinant of $L(t)$ is related to the pressure tensor in the same way as in Eq. (10).

4. APPLICATIONS OF PERIODIC ORBIT THEORY

As noted in the Introduction, the theory of unstable periodic orbits as a means of deriving stationary measures of Axiom A systems is well developed.[21,32,33] At least two kinds of these can be obtained through periodic orbits; indeed, unweighted orbital probability measures converge weakly to the measure of maximum topological entropy,[34] while orbital probability measures, weighted by the expanding eigenvalues of the associated stability matrices, converge weakly to the SRB measure.[22] We are interested in this second set of orbital measures, on the grounds of the predictive value of principle **R**.[16] As for the method of ref. 1, the stationary measure is not available in explicit form, but only indirectly through the averages of phase variables. This, we believe, is a typical situation for nonequilibrium steady states, which distinguishes them from (many) equilibrium ones.[27]

So far, the use of unstable periodic orbits (UPOs) for predictive purposes has been limited to low-dimensional dynamical systems, especially in the quantum chaos literature.[24] We show here possible ways of extending this approach to many-particle systems in nonequilibrium statistical mechanics. In order to do this, consider a system of the sort discussed in previous sections, and introduce a Poincaré section for it. This can be done by taking snapshots of the evolution at discrete times corresponding to collisions among particles. In the case of soft potentials a collision may be identified by the instant at which two or more particles come within a certain distance of each other. Then, let us assume that the natural measure of a given system can be approximated by unstable periodic orbits, that is, that principle **R** holds. The average of a phase variable $B(\mathbf{q}, \mathbf{p})$ in this case can be expressed as

$$\langle B \rangle = \lim_{m \to \infty} \frac{\sum_{i \in P_m} \Lambda_{1i}^{-1} \int_0^{\tau_i} B(s, s_{i0})\, ds}{\sum_{i \in P_m} \tau_i \Lambda_{1i}^{-1}} \tag{11}$$

where P_m is the set of UPOs with m collisions, Λ_{1i} is the product of the expanding eigenvalues of the stability matrix, and τ_i is the length of the ith UPO (here each orbit has been parametrized by the variable s, which is the distance traveled along the orbit from an arbitrary origin s_{i0}).

Naturally, expansion (11) would hold if the chaoticity assumption of Gallavotti and Cohen was satisfied. However, the numerical work on low-dimensional systems seems to indicate that the conditions on principle **R**

can be relaxed considerably[10,11,17,18,35] and this entails the possibility of extending the use of Eq. (11) beyond the limits of such a hypothesis. Indeed, the work by Chernov *et al.*[19] shows that for **R** to hold, smoothness of the flow is not always necessary, while our numerical simulations[11] indicate that Eq. (11) produces the correct results for one such system over a wide range of field magnitudes. Chernov *et al.*[19] also demonstrate that the initial ensemble does not necessarily need to be the Liouville measure: for the nonequilibrium Lorentz gas at small fields, it suffices to take an initial ensemble which is absolutely continuous with respect to such a measure. There are also speculations[32,14] (some based on numerical evidence[36]) that periodic orbit expansions do not need to be restricted to hyperbolic systems. Whether and how the chaoticity assumption can be relaxed according to these ideas and extended to thermostatted systems of many particles is, however, a matter of pure speculation at present, except for the (rather large) existing body of numerical results for systems of several particles. In particular, it is not known whether the observed agreement between periodic orbit expansion results and thermodynamic quantities is merely the effect of the limited accuracy of the numerical work (however, this seems to be a remote possibility). Thus the chaoticity assumption of Gallavotti and Cohen remains for the moment the most solid mathematical basis for our and similar arguments.

As a simple application of periodic orbit theory, let us compute the entropy production rate, σ say, for our systems. In particular, for the case of a fixed external field we have that σ equals $\mathbf{J} \cdot \mathbf{F}_e / T = J_x F_e / T$,[37] where $\mathbf{J}$ is the dissipative current and T is the fixed temperature of the system. Observe that the current associated with a periodic (up to lattice translations) orbit satisfies

$$-\int_0^{\tau_i} ds\, J_{xi}(s)\, F_e = kT \sum_{l=1}^{2dn} \lambda_{il} \tau_i$$

Therefore, using Eq. (11), we have

$$\sigma = \frac{\mathbf{J} \cdot \mathbf{E}}{kT} = -\lim_{m \to \infty} \frac{\sum_{i \in P_m} \tau_i \Lambda_i^{-1} \sum_{l=1}^{2dn} \lambda_{il}}{\sum_{i \in P_m} \tau_i \Lambda_i^{-1}} = -\left\langle \sum_{i=1}^{2dn} \lambda_i \right\rangle$$

Similarly, for the shear flow case the entropy production rate can be defined as the divergence of the right-hand side of the equations of motion, and, on average, it turns out to be

$$\sigma = \lim_{m \to \infty} \frac{\sum_{i \in P_m} \tau_i \Lambda_i^{-1} (1/\tau_i) \int_0^{\tau_i} \alpha(s)\, ds}{\sum_{i \in P_m} \tau_i \Lambda_i^{-1}} = -\left\langle \sum_{i=1}^{2dN} \lambda_i \right\rangle$$

In both cases, one can look at the probability that the total entropy production in a given interval of time is a certain amount, so to obtain a result related to the fluctuation theorem of Gallavotti and Cohen.[1] To do this, observe that the probability of a UPO with m collisions relative to all the UPOs with same number of collisions is given by

$$\pi_i = \frac{\tau_i \Lambda_{u,i}^{-1}}{\sum_{j \in P_m} \tau_j \Lambda_{u,j}^{-1}}$$

Because of the time reversibility of our systems, for every periodic orbit there is a second one of the same period whose stability eigenvalues are the inverse of those of the first; we regard these orbits as *conjugate*. In the case of a fixed external field, the two orbits share the same set of configuration points $\{\mathbf{q}(s)\}_{s=0}^{\tau}$, but their momenta at a point $\mathbf{q}$, $\mathbf{p}^+$ and $\mathbf{p}^- = -\mathbf{p}^+$, say, are opposite to each other. Thus, these two orbits give opposite contributions to the current of the system. In the case of shear flows the orbits with equal period and inverse stability eigenvalues are related in a more complicated way, that is, they can be transformed into each other by means of a *Kawasaki* mapping.[12] Such orbits contribute opposite off-diagonal terms to the pressure tensor.[3] The proportionality of the sum of Lyapunov exponents to the entropy production rate (related to the current in the case of fixed external field, and to the pressure tensor in the shear flow case) allows us to express the relative probability of a UPO with given entropy production to that of a UPO with opposite entropy production as

$$\frac{\pi_i}{\pi_{-i}} = \frac{\Lambda_{u,i}^{-1}}{\Lambda_{u,-i}^{-1}} = \Lambda_i^{-1} = \exp\left(-\tau_i \sum_l \lambda_{i,l}\right) = e^{c\sigma}$$

where c is a fixed constant, independent of i, for a given system. Then we may define the relative probability of finding a trajectory with given entropy production to that of a trajectory with opposite entropy production as the following limit:

$$\frac{\pi(\sigma)}{\pi(-\sigma)} = \lim_{m \to \infty} \frac{\sum_{i \in P_m(\sigma)} \pi_i}{\sum_{i \in P_m(-\sigma)} \pi_i}$$

$$= \frac{\sum_{i \in P_m(\sigma)} \tau_i \Lambda_{u,i}^{-1}}{\sum_{i \in P_m(-\sigma)} \tau_i \Lambda_{u,i}^{-1}} = \frac{\tau_1 \Lambda_{u,1}^{-1} + \tau_2 \Lambda_{u,2}^{-1} + \cdots}{\tau_1 \Lambda_{u,-1}^{-1} + \tau_2 \Lambda_{u,-2}^{-1} + \cdots} = e^{c\sigma} \qquad (12)$$

[3] Clearly, only in the case of nonvanishing current (off-diagonal terms of the pressure tensor) can we claim that conjugate orbits are distinct; otherwise one orbit may coincide with its conjugate.

where we used the fact that each pair of conjugate trajectories shares exactly the same period and that $\Lambda_{i,u}^{-1}/\Lambda_{-i,u}^{-1}=\Lambda_i^{-1}$. In Eq. (12), $P_m(\sigma)$ is the set of periodic orbits with m collisions and entropy production rate σ.

Similar manipulations can be used for determining some qualitative properties of the current or of the pressure tensor. For instance, we can organize all the periodic orbits with m collisions in three sets; let P_m^+ be the set of UPOs with positive current (pressure tensor), using the convention that the positive direction of the x axis is the same as the direction of the external field or of the shear. Let P_m^- be the set of UPOs with negative current (pressure tensor), and let P_m^0 be the set of those with vanishing current (off-diagonal pressure tensor).[4]

Assuming that the attractor of our system is of the kind described in ref. 1, e.g., it is Anosov-like, we have that if one UPO is embedded in it, its conjugate UPO is embedded in the attractor as well. Then, Eq. (11) can be rewritten as

$$\langle B\rangle = \lim_{m\to\infty}\frac{1}{C_m}\left[\sum_{i\in P_m^+}\Lambda_{1i}^{-1}\int_0^{\tau_i}B(s,s_{i0})\,ds + \sum_{i\in P_m^-}\Lambda_{1i}^{-1}\int_0^{\tau_i}B(s,s_{i0})\,ds + \sum_{i\in P_m^0}\Lambda_{1i}^{-1}\int_0^{\tau_i}B(s,s_{i0})\,ds\right] \tag{13}$$

where every orbit in the first sum has a conjugate counterpart in the second sum, and the normalization constant is

$$c_n=\sum_{i\in P_n}\tau_i\Lambda_{1i}^{-1}$$

If the phase variable B is the current for the case of fixed external field, or the off-diagonal term of the pressure tensor for the shear flow case, the integrals of B over conjugate orbits are equal in magnitude and opposite in sign (with vanishing contributions coming from the orbits in P_m^0). Therefore, introducing $\tau_i\langle B\rangle_i=\int_0^{\tau_i}B(s,s_{i0})\,ds$, and denoting by $-i$ the trajectory conjugate to i, we find that Eq. (13) takes the form

$$\begin{aligned}\langle B\rangle &= \lim_{n\to\infty}\frac{1}{c_n}\sum_{i\in P_n^+}\tau_i\langle B\rangle_i\left[\Lambda_{1i}^{-1}-\Lambda_{1,-i}^{-1}\right]\\ &= \lim_{n\to\infty}\frac{1}{c_n}\sum_{i\in P_n^+}\Lambda_{1i}^{-1}\tau_i\langle B\rangle_i\left[1-\Lambda_i\right]\end{aligned} \tag{14}$$

[4] It is interesting to note that the orbits in P_m^0 for which the integral of α over a period vanishes preserve phase-space volumes and produce no entropy, similar to the case of equilibrium trajectories.

where

$$\Lambda_i = \exp\left(-r\int_0^{\tau_i}\alpha(s, s_{i0})\,ds\right) = \exp(-\phi\tau_i\langle B\rangle_i)$$

Here, r is a positive constant given in Section 2 for $B=J$, and in Section 3 for $B=\sum_i p_{xi}p_{yi}/m_i$, while ϕ is related to either the external field or the shear rate, depending on the case. It follows that the sign of $\langle B\rangle$ is nonnegative because all terms in the expansion have the form $x(1-e^{-cx})$, where c is a positive constant. Similarly, if we reverse our convention and take positive the direction against the field (or against the shear), we find that $\langle B\rangle$ is nonpositive. This fact shows how macroscopic irreversibility emerges in our systems with reversible dynamics. Moreover, because the number of degrees of freedom is not specified, our result holds for large as well as small systems. Clearly our result depends on the choice of the invariant measure, of which there are infinitely many. However, our choice corresponds to the physical (natural) measure, and thus it is the relevant one for the thermodynamics of our systems.

5. CONCLUSIONS

With a few examples we have shown how periodic orbits might be used in the study of nonequilibrium many-particle systems without actually having to compute the properties of any one of them. In order to do this, we had to rely on features of the particles' dynamics which have not been rigorously established so far, but which are strongly supported by many numerical studies, including both direct and indirect tests of the relevant stationary measures and of the associated Lyapunov spectra. These facts lead to the conclusion that some form of the chaoticity assumption (or of principle **R**) of Gallavotti and Cohen is actually verified in the molecular dynamic simulations of nonequilibrium fluids subjected to different kinds of driving mechanisms. We can safely say this at least within the limits of accuracy attainable with present-day computing facilities. Thus, the use of unstable periodic orbits is justified in the construction of the nonequilibrium ensembles, which can be obtained as a weak limit of normalized, weighted orbital measures, where the weights are the inverses of the stability eigenvalues associated with such orbits. The corresponding SRB measures should be the limiting measures of the dynamics, at least for initial conditions which are sampled randomly with respect to the Liouville measure. This, indeed, is sufficient if the dynamics, as for Anosov systems, satisfies the Axiom A conditions, but we expect that more general situations can be considered.

Thus we are led to conclude that periodic orbit theory for many-particle systems is equivalent to the theory of ref. 1, as, in particular, it is equally parameter free and it reproduces the same nonequilibrium ensembles through appropriate limiting procedures. We also believe that the two methods are marred by similar and complementary difficulties in their numerical implementation, so that the use of one or the other for a given system may be more effective depending on the particular problem. As a matter of fact, a direct implementation of Eq. (6.3) of ref. 1 for a system with more than a few particles may be beyond present-day computer abilities, and the situation may not be different for the implementation of our Eq. (11). However, much work is being done on periodic orbit expansions aimed at increasing their numerical efficiency. Two approaches can be followed in this direction: the development of convergence acceleration methods, and the understanding of how just a few orbits of short period could be used for accurate approximations of the natural measure.[40] Because of these facts and of the growing speed of computers, we believe that the state of the art will improve considerably in the coming years. At the same time, rather than implementing the methods described in this paper and in ref. 1, other methods, like the one of ref. 15, could be used, as proposed by Gallavotti and Cohen.

We conclude by observing that for Axiom A flows the measure of maximum topological entropy, obtained as the weak limit of unweighted orbital measures, and the SRB measure can be reduced to coincide, under suitable conditions, by a unique transformation of the speed of the flow.[22] Thus, to investigate the question of the equivalence of those two measures for many-particle systems might be beneficial for the applicability of periodic orbit theory, as the whole theory would be simplified whenever such equivalence holds. This will also be mirrored in much simpler numerical work, as it will remove the need for the computation of stability eigenvalues. Moreover, in a recent work Tasaki and Gaspard[38] suggested that maximizing the (Kolmogorov–Sinai) entropy may provide a guiding principle in the choice of the stationary ensemble, so that thermodynamics naturally emerges.

Finally, the argument recently proposed to understand the origin of irreversible behavior in the Lorentz gas[26] has been shown to be applicable to N-particle systems. This extension only requires two properties of the system. The first is that the stability weight associated with each periodic orbit is equal to the product of the expanding Lyapunov numbers, and the second is that the Lyapunov sum rule is exactly satisfied for each periodic orbit. The mechanism can then be applied to any thermostatted N-particle system which has these two properties.

ACKNOWLEDGMENTS

We thank E. G. D. Cohen and G. Gallavotti for helpful remarks. Thanks are also in order to C. Grebogi for his comments on hyperbolicity, and to R. Artuso for remarks on periodic orbit expansions. This work has been supported by the Australian Research Council (A69131116 and A69530230). L.R. gratefully acknowledges partial support from GNFM-CNR (Italy).

REFERENCES

1. G. Gallavotti and E. G. D. Cohen, *Phys. Rev. Lett.* **74**:2694 (1995); *J. Stat. Phys.* **80**:931 (1995).
2. G. P. Morriss and L. Rondoni, *Aust. J. Phys.* **49**:51 (1996).
3. G. P. Morriss, *Phys. Lett.* **122A**:236 (1987); *Phys. Rev. A* **37**:2118 (1988); *Phys. Lett. A* **143**:307 (1989); *Phys. Rev. A* **39**:4811 (1989).
4. P. Gaspard, *J. Stat. Phys.* **68**:673 (1992); *Chaos* **3**:427 (1993).
5. D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic Press, London, 1990).
6. S. Sarman, D. J. Evans, and A. Baranyai, *Physica A* **208**:191 (1994).
7. H. A. Posch and W. G. Hoover, *Phys. Rev. A* **38**:473 (1988); G. P. Morriss, *Phys. Rev. A* **37**:2118 (1988).
8. D. J. Evans, E. G. D. Cohen, and G. P. Morriss, *Phys. Rev. A* **42**:5990 (1990).
9. B. Moran and W. G. Hoover, *J. Stat. Phys.* **48**:709 (1987).
10. W. N. Vance, *Phys. Rev. Lett.* **69**:1356 (1992).
11. J. P. Lloyd, M. Niemeyer, L. Rondoni, and G. P. Morriss, *Chaos* **5**:536 (1995).
12. G. P. Morriss and D. J. Evans, *Phys. Rev. A* **39**:6335 (1989).
13. E. G. D. Cohen, *Physica A* **213**:293 (1995).
14. P. Gaspard and F. Baras, *Phys. Rev. E* **51**:5332 (1995); J. R. Dorfman and P. Gaspard, *Phys. Rev. E* **51**:28 (1995); P. Gaspard and J. R. Dorfman, *Phys. Rev. E* **52**:3525 (1995).
15. D. J. Evans, E. G. D. Cohen, and G. P. Morriss, *Phys. Rev. Lett.* **71**:2401, 3616 (1993).
16. G. Gallavotti, *J. Stat. Phys.* **78**:1571 (1995).
17. G. P. Morriss and L. Rondoni, *J. Stat. Phys.* **75**:553 (1994).
18. G. P. Morriss, L. Rondoni, and E. G. D. Cohen, *J. Stat. Phys.* **80**:35 (1995).
19. N. I. Chernov, G. L. Eyink, J. L. Lebowitz, and Ya. G. Sinai, *Phys. Rev. Lett.* **70**:220 (1993); *Commun. Math. Phys.* **154**:569 (1993).
20. G. Gallavotti, Reversible Anosov diffeomorphisms and large deviations, preprint.
21. D. Ruelle, *Thermodynamic Formalism* (Addison-Wesley Reading, Massachusetts, 1978).
22. W. Parry, *Commun. Math. Phys.* **106**:267 (1986).
23. G. Gallavotti, personal communication.
24. Focus issue on periodic orbit theory, *Chaos* **2**(1) (1992).
25. P. Cvitanovic, The power of chaos, in *Applied Chaos*, J. H. Kim and J. Stringer, eds. (Wiley, New York, 1992), p. 413.
26. G. P. Morriss and L. Rondoni, Unpublished.
27. L. Rondoni and G. P. Morriss, *Phys. Rev. E* **53**:2143 (1996).
28. S. Goldstein, C. Kipnis, and N. J. Ianiro, *J. Stat. Phys.* **41**:915 (1985).
29. W. G. Hoover, *Molecular Dynamics* (Springer-Verlag, Berlin, 1986).
30. S. Sarman, D. J. Evans, and G. P. Morriss, *Phys. Rev. A* **45**:2233 (1992).

31. J.-P. Eckmann and D. Ruelle, *Rev. Mod. Phys.* **57**:617 (1985).
32. C. Grebogi, E. Ott, and J. A. Yorke, *Phys. Rev. A* **37**:1711 (1988).
33. R. Artuso, E. Aurell, and P. Cvitanovic, *Nonlinearity* **3**:325 (1990).
34. R. Bowen, *Am. J. Math.* **94**:413 (1972).
35. P. Cvitanovic, P. Gaspard, and T. Schreiber, *Chaos* **2**:85 (1992).
36. C. Grebogi, Personal communication.
37. L. E. Reichl, *A Modern Course in Statistical Physics* (Texas University Press, Austin, Texas, 1984).
38. S. Tasaki and P. Gaspard, Fractal distribution and Fick's law in a reversible chaotic system, in *Towards the Harnessing of Chaos*, M. Yamaguti, ed. (Elsevier, Amsterdam, 1994).
39. T. Tel, J. Vollmer, and W. Breymann, Transient chaos: The origin of transport in driven systems, preprint (1995).
40. R. Artuso, Personal communication.