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Chaotic Hypothesis: Onsager Reciprocity and Fluctuation-Dissipation Theorem

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It is shown that the chaoticity hypothesis recently introduced in statistical mechanics, which is analogous to Ruelle's principle for turbulence, implies the Onsager reciprocity and the fluctuation-dissipation theorem in various reversible models for coexisting transport phenomena.

KEY WORDS: Chaotic hypothesis; Ruelle principle; Onsager reciprocity; fluctuation dissipation.

1. INTRODUCTION

In ref. 25 we introduced as a principle, holding when the time evolution of a system has an empirically chaotic nature, the following:

Chaotic Hypothesis. A many-particle system in a stationary state can be regarded, for the purpose of computing macroscopic properties, as a smooth dynamical system with a transitive Axiom A global attractor. In the reversible case it can be regarded, for the same purposes, as a smooth transitive Anosov system.

In an attempt to make this paper more accessible, care has been taken to avoid, as much as possible, reliance on technical aspects of the theory of Anosov and Axiom A systems: a classical reference to this theory is ref. 44; for more specialized references see refs. 1, 42, 37–39, and 2 (for the

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This paper is dedicated to David Ruelle on the occasion of his 60th birthday.

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Anosov systems) and refs. 2 and 40 (for the more general systems with Axiom A attractors).[3]

The evolution of the system is described by differential equations of motion in phase space. To be concrete, one can keep in mind the simplest of the (two) classes of models (two-dimensional, for simplicity) that we consider in this paper. It is a model for diffusion in a mixture of two chemically inert gases whose $N = N_1 + N_2$ molecules (with equal masses m and respective numbers $N_1 = N_2$) are contained in a box $\mathscr{B} = [-\frac{1}{2}L, \frac{1}{2}L]^2$ with periodic boundary conditions. They are each subject to a respective external force field $\mathbf{E}^1 = E^1\mathbf{i}$ and $\mathbf{E}^2 = E^2\mathbf{i}$ in the x direction. The molecules interact via a pair interaction with a short-range potential (e.g., a hard-core or a Lennard-Jones potential) elastically colliding as well as with fixed circular obstacles. The latter are so arranged as to prevent straight-line trajectories in the absence of external fields.[4] The total force (including the impulsive force due to the obstacles) on the jth particle will be $\mathbf{F}_j$.

Furthermore, the motion is subject to the constraint that the total energy is constant, via a constraint force law which is *ideal* in the sense that it satisfies Gauss' principle of minimal constraint (see Appendix A1). This means that, if E_j is the field on the jth particle (equal either to E^1 or to E^2), the equations of motion are

$$\dot{\mathbf{q}}_j = \frac{1}{m}\mathbf{p}_j, \qquad \dot{\mathbf{p}}_j = \mathbf{F}_j + \mathbf{E}_j\mathbf{i} - \alpha\mathbf{p}_j \tag{1.1}$$

with $\alpha = \sum_j E_j\mathbf{i}\cdot\mathbf{p}_j/\sum_j \mathbf{p}_j^2$.

The motions described by (1.1) generate a flow $x \to V_t x$ in phase space so that the time evolution of an observable F on the trajectory starting at x is the function $t \to F(V_t x)$.

We are interested in the asymptotic properties of $F(V_t x)$ as $t \to \infty$ for the initial data x which can be obtained by a random selection with some probability distribution μ_0. In other words, we give an initial density distribution μ_0 on phase space and we want to study how it evolves in time.

The asymptotic properties will in general depend on the choice of μ_0 and the averages over the time variable t give the *stationary* state for the

[3] I do not known an example of a reversible system with an Axiom A transitive global attractor which, as a subsystem, is not a smooth manifold (hence an Anosov subsystem): in this sense the second part of the hypothesis is closely related to the first part, i.e., close to being a consequence of the first. However, in this paper the latter part of the hypothesis will be needed and is used in a literal sense: this is a too strong assumption at large forcing, but here we only consider small forcing; see ref. 4.

[4] This is used only to ensure that at least when the mutual interactions vanish the motion of each of the particles is "chaotic."[16] The total force (including the impulsive force due to the obstacles) on the jth particle will be $\mathbf{F}_j$.

evolution V_t, *provided they are uniquely defined*, i.e., provided that for almost all choices of x with distribution μ_0 the averages exist and are x independent. In the latter case the stationary state is a stationary probability distribution μ: to stress that it is *dependent on* μ_0 we call it the *statistics* μ of μ_0.

In many applications it is more convenient to regard the evolution as a discrete transformation defined on a restricted phase $\mathscr{C}$ of *observed events*, also called *timing events* (which could be, for instance, the occurrence of a microscopic binary "collision"). The time evolution, or the *dynamics*, then becomes a map S of $\mathscr{C}$ into itself. The map S is derived by solving the differential equations of motion of the system, which gives us a flow on phase space that will be called V_t: the timing events $\mathscr{C}$ have to be thought of as a surface transverse to the flow. If $t(x)$ is the time between the timing event x and the successive one Sx, then $V_{t(x)}x = Sx$. Note that, for the intermediate times, the points $V_t x$ *are not* timing events (i.e., they are not in $\mathscr{C}$) $0 < t < t(x)$.[5]

The notion of *statistics* μ of μ_0 carries over unchanged to the discrete evolution and the above chaotic hypothesis is assumed in such a context. When referring to phase space, unless stated otherwise, we think of a phase space $\mathscr{C}$ consisting of timing events and of a map S on $\mathscr{C}$ defining the time evolution. The *smoothness* of the Anosov system holds for all the coordinates and parameters on which the system equations depend.

The chaotic hypothesis implies, as a mathematical consequence, that *for most distributions* μ_0 *of the initial data* x the distribution μ exists. However, the choice of the initial data with distribution μ_0 *proportional to the volume measure on* $\mathscr{C}$ plays a special role, because in the case of Hamiltonian systems such a distribution is generated naturally via the microcanonical ensemble.

For instance, one can read that (translating symbols into the present notation),[(26)] "the appropriate objects of study of a statistical mechanics of time dependent phenomena are the random processes $F(V_t x)$ *with initial distribution of* x, $\rho_E(x)$ (*the microcanonical distribution*), for all energies of interest and for all gross variables F of interest" (italics added).[6]

[5] This is natural, as the observations are often timed by "remarkable" events, like events between which the system evolution can be exactly, or almost exactly, computed; technically this has the advantage of reducing the dimension of phase space by one unit and of eliminating a coordinate responsible for a zero Lyapunov exponent, which is always desirable, when possible.

[6] Although I disagree with elevating to a philosophical principle that the "interesting initial data" are those that one gets by selecting them with a distribution which is, as often said, "absolutely continuous with respect to the phase space volume," i.e., it is given by a density on phase space, I will adopt it here because it is obvious that, whether one agrees or not, it is *of fundamental interest* to understand the statistics of initial data chosen at random with a distribution proportional to the phase space volume. Other random choices may have to wait until the latter is properly understood.

In the physics literature the existence of the distribution μ is, in fact, assumed in general, very often (very) tacitly, but sometimes explicitly, and it can be stated formally as a "law" by the following (extension) of the zeroth law,[45] gibing a global property of the motions generated by initial data chosen randomly with distribution μ_0 proportional to the volume measure on $\mathscr{C}$:

Extended Zeroth Law. A dynamical system $(\mathscr{C}, S)$ describing a many-particle system (or a continuum such as a fluid) generates motions that admit a statistics μ in the sense that, given any (mooth) macroscopic observable F defined on the points x of the phase space $\mathscr{C}$, the time average of F exists for all μ_0-randomly chosen initial data x and is given by

$$\lim_{M \to \infty} \frac{1}{M} \sum_{k=0}^{M-1} F(S^j x) = \int_{\mathscr{C}} \mu(dx')\, F(x') \tag{1.2}$$

where μ is an S-invariant probability distribution on $\mathscr{C}$.

The chaotic hypothesis was proposed by Ruelle in the case of fluid turbulence, and it is extended to nonequilibrium many-particle systems in ref. 24. If one assumes it, then it *follows* that the zeroth law holds[42,2,37–40]; however, it is convenient to regard the two statements as distinct because the hypothesis we make is "*only*" that one can suppose that the system is Axiom A or Anosov for "practical purposes": this leaves open the possibility that it is not strictly speaking that such and some ("negligible in the thermodynamic limit") corrections may be needed to the predictions obtained by using the hypothesis.

From now on only reversible systems will be considered in this paper: they are dynamical systems such that there is an isometric map i of phase space such that $i^2 = 1$ and $iS = S^{-1}i$: note that in the case of (1.1) the *time reversal* transformation exists and it is simply the usual $i(\mathbf{q}, \mathbf{p}) = (\mathbf{q}, -\mathbf{p})$.

In ref. 25 the generality of the hypothesis is discussed and in refs. 24 and 25 we derived, as a rather general consequence, predictions testable by numerical experiment in systems with few degrees of freedom (by definition here few means "accessible to numerical experiments" designed for the specific purpose of testing the hypothesis, i.e., $\sim 10^2$). The most relevant feature of the prediction, which is a *large-deviation theorem* or *fluctuation theorem* for systems with reversible dynamics, is that it is *parameter free.* A drawback is that the prediction *is not* testable directly in really large systems ("real systems" with $\sim 10^{20}$ degrees of freedom).

From a historical point of view Ruelle's original proposal (1973 at least) and the question of whether the "chaotic hypothesis" could be tested on real experiments, even with few particles, remained open: the question was implicitly posed in ref. 16, but the first attempt at a test is in ref. 12, which contains a really new idea, subsequently made precise and developed in refs. 24 and 25.

In this paper we show, through examples, that the chaotic hypothesis implies quite generally, in systems with reversible dynamics, the Onsager reciprocity and the fluctuation-dissipation theorem: see ref. 9 for a classical general discussion of the reciprocity relations, see ref. 5, Appendix A, pp. 187–200, and ref. 43 for a kinetic derivation; see also refs. 10, 13, and 29 for recent developments. A very nice introduction and an exposition of the basic ideas can be found in ref. 8. The ideas of the present paper can be applied also to systems relevant for the theory of developed turbulence.[22]

In Sections 2 and 3 we introduce the models which will be used to illustrate our general ideas; in Section 4 we discuss the relevant mathematical facts about reversible Anosov systems and derive the basic expression for the Sinai–Bowen–Ruelle distribution (SRB distribution), which shows that the latter can be considered as the nonequilibrium analog of the equilibrium ensembles (as its expression bears a striking analogy with the familiar Boltzmann Gibbs distributions described by suitable weights on phase space cells).

The models we consider share the following properties:

1. They depend on parameters measuring the size of external driving forces (which may be reversible force fields or temperature differences) which we call $\mathbf{e} = (a, b, c, \ldots)$.

2. They have a reversible thermostatting mechanism that keeps the energy from growing.

3. They have a variation per unit time of the phase space volume described by a function $\sigma(x)$ on phase space that can be naturally identified with an *entropy generation* per unit time.

Hence in our models one can *unambiguously* identify the *thermodynamic forces* $\mathbf{e}$ and the conjugate *flows* $\mathbf{j}$, because there is a well-defined microscopic entropy generation rate σ to be used in the defining relation[9]:

$$j_z = \langle \partial_z \sigma \rangle_{\mathbf{e}}, \qquad z \in \mathbf{e} = (a, b, c, \ldots) \tag{1.3}$$

where $\langle \cdot \rangle_{\mathbf{e}}$ denotes the average with respect to the statistics μ for the motions developing in the fields $\mathbf{e}$. While the above definition is in principle different from the microscopic definition of flow, corresponding more to a macroscopic description, we expect them to coincide. This is indeed the case here, as can be seen from (5.11) below.

On a heuristic basis one accepts *a priori* that in time-reversible systems the phase space contraction rate is proportional to the entropy creation rate.[1] Then (1.3) acquires a remarkable generality: it allows us to define the *conjugate pairs* of thermodynamic forces and thermodynamic flows, by combining the well-known Onsager prescription with the definition in ref. 41. If the thermodynamic forces are actually identical to external forces acting on the system (rather than just functions of them, as is usual in many shear flow models[12,7]) then σ should be expected to be necessarily the sum of the products of the currents J_z divided by $k_B T$ times the forces z: $\sigma = \sum_z (J_z/k_B T) z$; this should make the agreement between (1.3) and what one would expect look less miraculous; see (5.11) below. In particular, this applies to thermostatted systems, which can be regarded as limits of Gaussian thermostats as in the shear flow models of refs. 12 and 7.

The label $\mathbf{e}$ in the relation $j_a = \langle \partial_a \sigma \rangle_{\mathbf{e}}$ stresses that the quantity j_a is evaluated at nonzero external forces $\mathbf{e}$ so that the time average will depend on the value of such forces and it will coincide (with probability 1, by the extended zeroth law) with the average with respect to the stationary distribution appearing in (1.2), i.e., the SRB distribution.

Then it makes sense to define the coefficients $L_{a,b} = \partial_b j_a|_{\mathbf{e}=\mathbf{0}}$ and to ask whether the Onsager relations hold, i.e., whether

$$L_{a,b} = \partial_b j_a|_{\mathbf{e}=\mathbf{0}} \stackrel{?}{=} \partial_a j_b|_{\mathbf{e}=\mathbf{0}} = L_{b,a} \tag{1.4}$$

Note that evaluating the derivatives of j requires considering the averages defining j_a, j_b in *nonvanishing external forces* $\mathbf{e} \neq \mathbf{0}$, hence it requires using the SRB distribution, and all the information that we have on it derives from the above chaotic hypothesis.

In Section 5, I give a proof, whose full mathematical rigor still rests on a mathematical conjecture (Section 5) on Anosov systems (that I hope to address elsewhere), of the validity of the fluctuation-dissipation relation and of the above Onsager reciprocity in the models introduced in Sections 2 and 3. The generality of the argument, which seems largely model independent, will also emerge.

Thus, at least in the models considered, the Onsager reciprocity holds as a consequence of the chaotic hypothesis: I regard this *not* as a better derivation of reciprocity, but rather as a further *confirmation* of the validity of the chaotic hypothesis (at least in the models considered). The Onsager reciprocity is one of the few noncontroversial results in nonequilibrium statistical mechanics: therefore it is reassuring that it is in some sense built into the chaotic hypothesis as well, since the latter has the ambition of representing a general law. It can thus be used in a way analogous to the heat theorem of Boltzmann,[18] which he employed to test the "correctness" of mechanical models of thermodynamics (a concept that he called *orthodicity* and that seems to have fallen into oblivion[18]).

Comments and a brief comparison with the classical derivations (that apply to our models as well) are presented in Section 6.

2. A DIFFUSION PROBLEM

We consider a mixture of two chemically inert gases introduced as the example described in Section 1; see (1.1).

The future time average of the total momentum **P** and of the dissipation α, considered after (1.1), $\langle \mathbf{P} \rangle_+ \neq 0$ and $\langle \alpha \rangle_+ \geqslant 0$[41] and expected to be nonzero if $(E^1, E^2) \neq 0$,[41] are expected to be attained exponentially fast, while the "conjugate" variable **C**, the center-of-mass position, will be expected to evolve with zero Lyapunov exponent (and to behave asymptotically as $\langle \mathbf{C} \rangle_+ = [1/(N_1+N_2)m] \langle \mathbf{P} \rangle_+ t + \text{const}$).

The phase space contraction per unit time is

$$\gamma = [2(N_1+N_2)-1]\alpha \tag{2.1}$$

We call Q the work per unit time performed by the forces $\alpha \mathbf{p}_j$, so that the phase space contraction rate in the configuration x is (to leading order in N) $2N\alpha(x)$, i.e.,

$$\frac{E^1 N_1 \dot{a}_1(x) + E^2 N_2 \dot{a}_2(x)}{k_B T(x)} = \frac{Q}{k_B T}$$

where k_B is Boltzmann's constant, $k_B T(x)$ is the kinetic energy per particle, $a_1(x)$, $a_2(x)$ are the horizontal coordinates of the centers of mass $\mathbf{C}_1$, $\mathbf{C}_2$ of the two species, and $\dot{a}_1(x)$, $\dot{a}_2(x)$ are the corresponding velocities. Thus the phase space contraction rate can be interpreted as $1/k_B$ times the *entropy creation rate* (at least if E^1, E^2 are so small that the center-of-mass horizontal velocities are small compared to the root mean square velocities).

We expect that the future time average of the total momentum **P** and of the dissipation α wil be some $\langle \mathbf{P} \rangle_+ \neq 0$ and $\langle \alpha \rangle_+ > 0$ if $(E^1, E^2) \neq 0$. It is reassuring that such a property can be rigorously established in the models studied in ref. 6 (one thermostatted particle only, interacting wih fixed obstacles and a constant field) at small forcing. Furthermore, it is possible to prove on rather general grounds that $\langle \alpha \rangle_+ \geqslant 0$, see [41], in systems including the ones considered here.

The above model is closely related to the *color diffusion* model considered in ref. 3. A *very* important feature of the model is its *time reversibility*: the map $i(\mathbf{p}, \mathbf{q}) = (-\mathbf{p}, \mathbf{q})$ has the property that it is an isometry of phase space such that $iS = S^{-1}i$ and $i^2 = 1$.

3. A HEAT CONDUCTION–ELECTRICAL CONDUCTION MODEL

As a second model, we consider a modification of model 4 of ref. 25, inspired by ref. 30; see also ref. 36 for a more general perspective on constrained systems. This is a model for a heat conducting and electrically conducting gas. In a box $\mathscr{B} = [-2L - H, 2L + H] \times [-L, L]$ (the dimensions are arbitrary and no special meaning should be attached to them, they merely reflect the shape drawn in Fig. 1) are enclosed N particles with mass m, interacting via a rather general pair potential, like a hard-core potential with a tail or via a Lennard-Jones potential, and they are subject to a constant force field (*electric field*) $E\mathbf{i}$ in the x direction; as in the previous model the particles also collide with fixed obstacles so arranged that no collisionless straight path can exist. The boundary conditions are periodic in the horizontal direction and reflecting in the vertical direction.

Adjacent to the box $\mathscr{B}$ there are two boxes $\mathscr{R}_+$, $\mathscr{R}_-$ containing $N_+ = N_-$ particles interacting with each other via a hard-core interaction and with the particles in $\mathscr{B}$ via a pair interaction (e.g., with potential equal to the one between the particles in $\mathscr{B}$), but are separated from the latter by a reflecting wall. The sizes and the location of the three boxes can be changed as one wishes and they are fixed only for definiteness.

The model name is motivated because we imagine other forces to act on the system: they are the minimal forces (in the sense of Gauss' minimal constraint principle, see Appendix A) necessary to enforce the following constraints:

1. The total kinetic energy in the "hot plate" $\mathscr{R}_+$ and that in the "cold plate" $\mathscr{R}_-$ are constrained to be $N_+ k_B T_+$ and $N_- k_B T_-$, respectively, where T_- and $T_+ = T_- + \delta T$, $\delta T \geqslant 0$, are the *temperatures of the plates*.

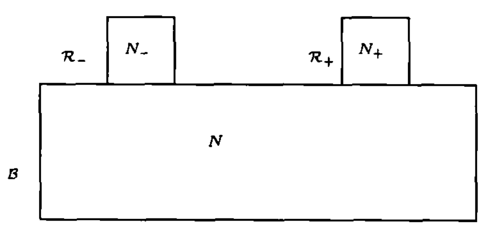

Fig. 1.

2. The total energy U in the box $\mathscr{B}$ is constrained to stay constant.

The equations of motion are, assuming hard core pair forces $\mathbf{F}_j$:

$$\begin{aligned} \dot{\mathbf{q}}_j &= \frac{\mathbf{p}_j}{m} \\ \dot{\mathbf{p}}_j &= \mathbf{F}_j + E\chi(\mathbf{q}_j)\,\mathbf{i} - \alpha_+\chi_+(\mathbf{q}_j)\,\mathbf{p}_j - \alpha_-\chi_-(\mathbf{q}_j)\,\mathbf{p}_j - \alpha\chi_{\mathscr{B}}(\mathbf{q}_j)\,\mathbf{p}_j \end{aligned} \tag{3.1}$$

where $\chi_{\mathscr{B}}$ and $\chi_\pm$ are the characteristic functions of the regions $\mathscr{B}$ and $\mathscr{R}_\pm$ and $\alpha_+\alpha_-$ and α are multipliers defined so that for some $T_\pm$

$$\sum_{j=1}^{N_\pm} \chi_\pm(\mathbf{q}_j)\,\frac{\mathbf{p}_j^2}{2m} = N_\pm k_{\rm B} T_\pm, \qquad \sum_{j=1}^{N} \chi_{\mathscr{B}}(\mathbf{q}_j)\,\frac{\mathbf{p}_j^2}{2m} = U \tag{3.2}$$

are exact constants of motion, $U = Nk_{\rm B}T_-$.

We suppose for simplicity (see, however, Remark 1 in Section 6) that the system in $\mathscr{B}$ is kept at a constant total energy U and at constant reservoir temperatures $T_\pm$. In this case call Q_+, Q_-, and Q_0 the work per unit time performed by the forces $\alpha_+\chi_+\mathbf{p}_j$, $\alpha_-\chi_-\mathbf{p}_j$, and $\alpha\chi\mathbf{p}_j$, respectively.

Let $\mathscr{L}_E$, $\mathscr{L}^0_+$, $\mathscr{L}^0_-$, $\mathscr{L}_+$, and $\mathscr{L}_-$ denote, respectively, the work per unit time performed by the field E or by the particles in the thermostats $\mathscr{R}_+$, $\mathscr{R}_-$ on the gas in $\mathscr{B}$, or by the gas in $\mathscr{B}$ on the thermostats $\mathscr{R}_+$, $\mathscr{R}_-$. Then the imposed conservation laws give

$$\begin{aligned} -Q_0 + \mathscr{L}_E + \mathscr{L}_+ + \mathscr{L}_- = 0 &\leftrightarrow U = \text{const} \\ -Q_+ + \mathscr{L}^0_+ = 0 &\leftrightarrow \sum_{\mathbf{q}_j\in\mathscr{R}_+} \frac{\mathbf{p}_j^2}{2m} = N_+ k_{\rm B} T_+ \\ -Q_- + \mathscr{L}^0_- = 0 &\leftrightarrow \sum_{\mathbf{q}_j\in\mathscr{R}_-} \frac{\mathbf{p}_j^2}{2m} = N_- k_{\rm B} T_- \end{aligned} \tag{3.3}$$

so that one easily finds [by differentiating (3.2) with respect to time and by applying the equations of motion (3.1)] expressions for α_+, α_-, α:

$$\begin{aligned} \alpha &= \frac{\mathscr{L}_E + \mathscr{L}_+ + \mathscr{L}_-}{\sum_{\mathbf{q}_j\in\mathscr{B}} \mathbf{p}_j^2/m} = \frac{Q_0}{\sum_{\mathbf{q}_j\in\mathscr{B}} \mathbf{p}_j^2/m} \\ \alpha_\pm &= \frac{\mathscr{L}^0_\pm}{2N_\pm k_{\rm B} T_\pm} = \frac{Q_\pm}{2N_\pm k_{\rm B} T_\pm} \end{aligned} \tag{3.4}$$

and the phase space contraction per unit time, or $1/k_B$ times the *entropy creation per unit time*, is in the configuration x

$$\gamma(x) = (2N_{\pm} - 1)(\alpha_+ + \alpha_-) + (2N - 1)\alpha \tag{3.5}$$

A key remark (J. Lebowitz, private communication) is that $\gamma \equiv 0$ if $E = J_+ - J_- = 0$.

The above model also shares the feature that it is *time reversible*, and the isometric map $i(\mathbf{p}, \mathbf{q}) = (-\mathbf{p}, \mathbf{q})$ is again such that $iS = S^{-1}i$ and $i^2 = 1$.

4. THE SRB DISTRIBUTION

The chaotic hypothesis of Section 2 allows us to represent the SRB distribution in a simple form, by using *Markov partitions*.[42] We consider *only* transitive reversible Anosov systems, although many concepts make sense for more general systems with chaotic attractors.

The notion of Markov partition is a mathematically precise version of the intuitive idea of *coarse graining*. We just recall here the main properties of Markov partitions. For a discussion of the intuitive meaning and the connection with the coarse graining see refs. 21 and 4.

1. A parallelogram will be a small set with a boundary consisting of pieces of the stable and unstable manifolds of the map S joined together as described below. The smallness has to be such that parts of the manifolds involved look essentially "flat": i.e., the sizes of the sides have to be small compared to the smallest radii of curvature of the *unstable manifolds* $W^u(x) \equiv W^u_x$ or of the *stable manifolds* $W^s(x) \equiv W^s_x$ as x varies in $\mathscr{C}$.

Therefore let δ be a length scale small compared to the minimal (among all x) curvature radii of the stable and unstable manifolds. Let Δ^u and Δ^s be small (and "small" means of size $\ll \delta$) connected surface elements on $W^u(x)$ and $W^s(x)$ containing x. We define a *parallelogram* E in the phase space $\mathscr{C}$, to be denoted by $\Delta^u \times \Delta^s$, with center x and axes Δ^u, Δ^s as follows.

Consider $\xi \in \Delta^u$ and $\eta \in \Delta^s$ and suppose that the point z, denoted $\xi \times \eta$, such that the shortest path joining ξ and η formed by a path on the stable manifold W^s_ξ joining ξ to z and by a path on the unstable manifold W^u_η joining z to η, is uniquely defined. This will be so if δ is small enough and if Δ^u, Δ^s are small enough compared to δ as we assume (because the stable and unstable manifolds are "smooth" and transverse).

The set $E = \Delta^u \times \Delta^s$ of all the points generated in this way when ξ, η vary arbitrarily in Δ^u, Δ^s is called a parallelogram (or rectangle), provided the boundaries $\partial\Delta^u, \partial\Delta^s$ of Δ^u and Δ^s as subsets of $W^u(x)$ and $W^s(x)$, respectively, have zero surface area on the manifolds on which they lie. The sets $\partial_u E \equiv \Delta^u \times \partial\Delta^s$ and $\partial_s E = \partial\Delta^u \times \Delta^s$ will be called the *unstable* or horizontal and *stable* or *vertical* sides of the parallelogram E.

Consider a partition $\mathscr{E}=(E_1,..., E_{\mathscr{N}})$ of $\mathscr{C}$ into $\mathscr{N}$ rectangles E_j with pairwise disjoint interiors. We call $\partial_u \mathscr{E} \equiv \bigcup_j \partial_u E_j$ and $\partial_s \mathscr{E} \equiv \bigcup_j \partial_s E_j$ respectively the *unstable boundary* of $\mathscr{E}$ and the *stable boundary* of $\mathscr{E}$, or also the horizontal and vertical boundaries of $\mathscr{E}$, respectively.

2. We say that $\mathscr{E}$ is a *Markov partition* if the transformation S acting on the stable boundary of $\mathscr{E}$ maps it into itself (this means $S\partial_s \mathscr{E} \subset \partial_s \mathscr{E}$) and if, likewise, the map S^{-1} acting on the unstable boundary maps it into itself $(S^{-1}\partial_u \mathscr{E} \subset \partial_u \mathscr{E})$.

The actual construction of the SRB distribution then proceeds from the important result of the theory of Anosov systems expressed by a remarkable theorem.[2]

Theorem. Every Anosov system admits a Markov partition $\mathscr{E}$.

Comments. (a) If the reversibility property holds, it is clear that $i\mathscr{E}$ is also a Markov partition. This follows from the definition of Markov partition and from the fact that reversibility implies

$$W_x^s = i W_{ix}^u \tag{4.1}$$

(b) The definition of a Markov partition also implies that the intersection of two Markov partitions is a Markov partition; hence it is clear that if a transitive Anosov system is reversible (i.e., there is an isometry i such that $iS=S^{-1}i$ and $i^2=1$), there are Markov partitions $\mathscr{E}$ that are reversible in the sense that $\mathscr{E}=i\mathscr{E}$, i.e., if $E_j \in \mathscr{E}$, there is j' such that $iE_j = E_{j'} \in \mathscr{E}$.

(c) The usefulness of the Markov partitions comes from the possibility that they provide of representing the points of $\mathscr{C}$ as *infinite strings* of symbols (in a more useful way than representing them, for instance, as the strings of digits that give the value of their coordinates).

This is simply achieved by associating with $x \in \mathscr{C}$ the string $\mathbf{j} = \{j_k\}_{k=-\infty}^{\infty}$ such that $S^k x \in E_{j_k}$. The invertibility of the map between $x \in \mathscr{C}$ and the *compatible* or *allowed* sequences, i.e., the sequences $\mathbf{j}$ such that the interior of SE_{j_k} intersects the interior of $E_{j_{k+1}}$ is a well known (and easy) consequence of the definition of Markov partition. The correspondence is in fact one to one with some obvious exceptions: namely, to each sequence $\mathbf{j}$ with the above compatibility property there corresponds one x; conversely, if x is not on a boundary of some of the $E \in \mathscr{E}$ nor on the image of a boundary under a power of S, then x admits only one symbolic representation. The points on the boundaries or visiting, in their evolution, the boundaries of course have several (but finitely many) symbolic representations, just in the same way as the decimal representation of a number is unique for most numbers: the ones which end with infinitely many successive 9's admit two representations.

The correspondence $x \leftrightarrow \mathbf{j}$ between points $x \in \mathscr{C}$ and their history, or symbolic representation, $\mathbf{j}$ as a compatile sequence will be denoted $x = x(\mathbf{j})$ (*symbolic code*).

(d) If we define the *compatibily matrix*, or *intersection matrix*, C_{ij} by setting $C_{ij} = 1$ in the interior of E_j intersects the interior of SE_i and $C_{ij} = 0$ otherwise, then the assumed transitivity implies that there is an iterate q of C such that all elements of C^q are positive (i.e., $S^q E_j$ has interior intersecting E_k for all pairs j, k simultaneously).

(e) Consider the partition $\mathscr{E}_M = \bigcap_{-M}^{M} S^{-j} \mathscr{E}$ obtained by intersecting the images under S^k, $k = -M,..., M$, of $\mathscr{E}$. Then $\mathscr{E}_M$ is still a Markov partition and it is time-reversal invariant if $\mathscr{E}$ is [see (b) above]. Note that the parallelograms of $\mathscr{E}_M$ can be labeled by the strings of symbols $j_{-M},..., j_M$ and they consist of the points x such that $S^k x \in E_{j_k}$ for $-M \leqslant k \leqslant M$. In other words, the parallelograms consists of those points x which, in their time evolution, visit at time k the parallelogram E_{j_k}.

(f) If $F(x)$ is a function on phase space (*observable*), then we can regard it as a function $F(x(\mathbf{j}))$ on symbolic sequences. An observable F is *local* if it "depends exponentially little" on the history symbols j_k with large k: i.e., if $F(x(\mathbf{j})) - F(x(\mathbf{j}'))$ tends to zero exponentially fast with the maximum number k such that $\mathbf{j}$ and $\mathbf{j}'$ agree on the sites with label h with $|h| \leqslant k$. A simple condition on F guaranteeing its locality is that F is Hölder continuous in x.

We now construct a probability distribution on $\mathscr{C}$ by defining it as a probability distribution on the space of the compatible strings $\mathbf{j}$ and then by interpreting it as a distribution on the phase space $\mathscr{C}$.

1. For this purpose we first pick a point, which we call the *center*, $x_{j_{-M},...,j_M}$ in each $E_{j_{-M},...,j_M}$ with nonempty interior simply by considering the compatible string which is obtained by continuing the string $j_{-M},..., j_M$ "to the right" into a string $j_M, j_{M+1},...$ and to the "left" into a string $..., j_{-M-1}, j_{-M}$ in a such way that the whole string $\mathbf{j}$ is compatible (i.e., such that there is a point x such that $S^k x \in E_{j_k}$ for all k) and, *furthermore*, the entries of the continuation strings *depend only* on the value of j_M and j_{-M}, respectively.

In general, given $j_{\pm M}$, there will be many choices of the continuation strings: which one we actually take is irrelevant. We impose, however, the further constraint that the continuation is made in a "time-reversible way," i.e., we choose the continuations so that if x is the center of E_j, then ix is the center of iE_j. A further restriction (not necessary in the following, but very natural) that one could consider is imposing that the continuation string to the right of j_M or to the left of j_{-M} agree identically after finitely many steps. Note that the existence of the continuation strings and the possibility of imposing the above restrictions on them are immediate consequences of the transitivity property of the compatibility matrix C.

2. We then define, given $\tau > 0$,

$$\bar{\Lambda}_{\mathrm{u},\tau}(x) = \prod_{j=-\tau/2}^{\tau/2-1} \Lambda_{\mathrm{u}}(S^j x) \tag{4.2}$$

where $\Lambda_{\mathrm{u}}(x)$ is the *local expansion coefficient* of the surface element of the unstable manifold at x, i.e., it is the Jacobian determinant of the transformation S regarded as a map of W^{u}_x into W^{u}_{Sx}. Likewise we define $\Lambda_{\mathrm{s}}(x)$ and $\bar{\Lambda}_{\mathrm{s},\tau}(x)$ as the corresponding quantities obtained by regarding S as a map of the stable manifold W^{s}_x to W^{s}_{Sx}.

3. Finally we define a distribution $\mu_{M,\tau}$ on $\mathscr{C}$ by "giving" to each set $E_{j_{-M},\ldots,j_M} \in \mathscr{E}_M$ a probability proportional to

$$\bar{\Lambda}^{-1}_{\mathrm{u},\tau}(x_{j_{-M},\ldots,j_M})\, \delta^{-1}_{\tau}(x_{j_{-M},\ldots,j_M})$$

where

$$\delta(x) \stackrel{\mathrm{def}}{=} \sin \vartheta(x) = \delta_0(x)$$

is the sine of the angle between the stable and the unstable manifolds at x and $\delta_\tau(x) = \delta(S^{\tau/2}x)$.

More precisely, we define the distribution $\mu_{M,\tau}$ so that the integral of a smooth function F is

$$\int_{\mathscr{C}} \mu_{M,\tau}(x)\, F(x) \stackrel{\mathrm{def}}{=} \frac{\sum_j \bar{\Lambda}^{-1}_{\mathrm{u},\tau}(x_j)\, \delta^{-1}_{\tau}(x_j)\, F(x_j)}{\sum_j \bar{\Lambda}^{-1}_{\mathrm{u},\tau}(x_j)\, \delta^{-1}_{\tau}(x_j)} \tag{4.3}$$

where j is a shorthand notation for $j_{-M},\ldots, j_M$ and $x_j = x_{j_{-M},\ldots,j_M}$ is the "center" chosen above in $E_j \in \mathscr{E}_M$. No relation is assumed here between M and τ, although in the applications we shall (naturally) taken $M = \tau/2$, as this simplifies the discussion considerably.

The distribution $\mu_{M,\tau}$ is very interesting because it is an approximation (a very good one) of the SRB distribution. In fact in refs. 14, 24, and 25 the following theorem is shown to be a reformulation (convenient, although trivially equivalent) of a basic theorem by Sinai:

Theorem. If $(\mathscr{C}, S)$ is a transitive Anosov system, the SRB distribution μ exists and the μ average of a local function [see (f) above] F is

$$\int_{\mathscr{C}} \mu(dx)\, F(x) = \lim_{M \to \infty, \tau \to \infty} \int_{\mathscr{C}} \mu_{M,\tau}(dx)\, F(x) \tag{4.4}$$

Furthermore, in (4.3) the factor $\delta_{\tau}^{-1}(x_j)$ could be replaced by $\delta_{\tau}^{z}(x_j)$ with z any pre-fixed real number (e.g., $z=0$). The limits can be interchanged.

The original statement is that μ exists and it is a Gibbs state with potential $\log \Lambda_{\mathrm{u}}^{-1}(x)$: see refs. 2, 37–40, and 42 for a discussion of this form of the statement. In ref. 40 the latter statement is extended to cover the case in which $(\mathscr{C}, S)$ has a global transitive Axiom A attractor: the discussion in refs. 19 and 20 shows that the above theorem extends, unchanged, to such cases. The extra factor δ_{τ}^{z} with $z=-1$ was absent in refs. 24 and 25, where z was chosen equal to 0 (an admissible alternative choice).

The possibility of fixing z arbitrarily, in spite of the apparently strong modification it introduces, is easily seen by examining the proof of (4.4).[19,20] The proof is based on the interpretation of (4.3) as a probability distribution on the space of the compatible strings. In this interpretation one immediately recognizes that (4.3) corresponds to a finite-volume Gibbs distribution for a suitable short-range Hamiltonian defined on the space of compatible strings. An extra factor $\delta_{\tau}^{z}(x_j)$ corresponds to considering the same Gibbs distribution *just with a different bounary condition*, which becomes irrelevant in the limit as $\tau \to \infty$ because one-dimensional Gibbs states with short-range interactions do not have phase transitions and therefore are insensitive to changes in the boundary conditions. Different choices of the center points also correspond to different choices of boundary conditions.

The choice $z=-1$ is much better than $z=0$ because it leads to simpler formulas and arguments: we shall call (4.3) a *balanced* approximation to the SRB distribution because, as we shall see, it is *reminiscent* of a probability distribution satisfying the detailed balance (which, however, is *not* satisfied in our models, except in zero forcing, i.e., in equilibrium).

In (4.4) with $M \gg \tau/2$ the choice of the point x_j in the parallelograms of $\mathscr{E}_M$ can be arbitrary, and it does not matter that x_j is really chosen as said above or just *anywhere* in $E_{j_{-M},\ldots,j_M}$ [because the variation of the weights (4.2) is in this case negligible, provided $M-\tau/2 \to \infty$ fast enough].

The extra properties that we need are that $\mathscr{E}_M$ is reversible (see above), i.e., $iE_j = E_{j'} \in \mathscr{E}_M$ (for a suitable j') and that, as a consequence of the reversibility [via (4.1) and the isometric nature of the time reversal map i and the validity of $\gamma(x) = -\gamma(ix)$ for the underlying differential equations],

$$\Lambda_{\mathrm{u},\tau}(ix) = \Lambda_{\mathrm{s},\tau}^{-1}(x), \qquad \delta_0(x) = \delta_0(ix), \qquad \delta_\tau(x) = \delta_{-\tau}(ix) \tag{4.5}$$

which are identities[25]; for the definitions of Λ_s, $\bar{\Lambda}_{s,\tau}$ see the lines following (4.2). Furthermore, the volume measure and the expansion and contraction rates are related by

$$\bar{\Lambda}_{u,\tau}(x)\,\bar{\Lambda}_{s,\tau}(x)\,\bar{\Lambda}_{s,\tau}(x)\,\frac{\delta_\tau(x)}{\delta_{-\tau}(x)} \equiv e^{-\tau t_0 \bar{\sigma}_\tau(x)} \tag{4.6}$$

where t_0 is the average time interval between successive timing events and the phase space volume contraction for a single transformation is written $e^{-t_0\sigma(x)}$, thus *defining* $\sigma(x)$ and $\bar{\sigma}_\tau(x)$:

$$\bar{\sigma}_\tau(x) \stackrel{\text{def}}{=} \frac{1}{\tau} \sum_{r=-\tau/2}^{\tau/2-1} \sigma(S^r x) \tag{4.7}$$

The condition (4.6) is obtained from the relation $\Lambda_u(x)\,\Lambda_s(x)\,\delta(Sx)/\delta(x) = e^{-t_0\sigma(x)}$ by evaluating it on the points $S^k x$, $k = -\tau/2,..., \tau/2 - 1$ and multiplying the results.

If the time interval $t(x)$ between the timing event $x \in \mathscr{C}$ and the successive one is very small and if its fluctuations can be neglected together with those of $\gamma(x)$ [see (2.1), (3.5)] (within the same time interval), then one simply has $\sigma(x) = \gamma(x)$. Note that *in all cases* with any reasonable definition of timing events the time $t(x)$ will tend to zero in the thermodynamic limit [as $O(N^{-1})$], but also γ will tend to infinity as $O(N)$.

More generally there is a simple relation between the function $\sigma(x)$ above and the function $\gamma(x)$ which describes the phase space contraction rate in the differential equations giving rise to the map S [see (2.1), (3.5)], namely

$$\sigma(x) = \frac{1}{t_0} \int_0^{t(x)} \gamma(Q_t x)\, dt \tag{4.8}$$

But the use of (4.8) is quite clumsy and one can always think that the timing events are chosen, artificially, much closer than the natural $t_0 = O(1/N)$ and observed at constant time intervals so that no difference really exists between $\gamma(x)$ and $\sigma(x)$. If necessity arises one can always use the precise relation (4.8), at the expense of some formal algebraic complications in the intermediate steps of our fothcoming deductions.

5. APPLICATIONS TO THE MODELS. ONSAGER RECIPROCITY, FLUCTUATION-DISSIPATION THEOREM

In this section we neglect for simplicity of exposition the difference between $\sigma(x)$ and $\gamma(x)$, i.e., we suppose that $t(x) = t_0$ is constant and that

γ is constant on the path traveled in the time interval $t(x)$: this simplifies the algebra considerably and the reader should have no trouble checking that the proper relation (4.8) could be consistently used leading to no corrections to the final results below (because in the end we shall set $\mathbf{E}=\mathbf{0}$).

Relation (4.3) has the form of a statistical average and we shall try to use it in the "same" way as in equilibrium statistical mechanics. We shall first study here the two currents J_h, $h=1,2$, generated by the pair of fields E_h in the diffusion model of Section 2.

The two currents are, where ρ_h and v_h are, the density and average velocity of the species h,

$$J_h=\rho_h v_h=\frac{N_h}{L^2}\frac{\sum_{j\in\{h\}}\mathbf{p}_j\cdot\mathbf{i}}{N_h m}=\frac{\sum_j \mathbf{p}_j^2/m}{L^2(2N-1)}\partial_{E_h}\sigma \tag{5.1}$$

where $j\in\{h\}$ means that j is a species-h particle, quantities of $O(N^{-1})$ have been neglected [see (2.1)], and σ is $1/k_B$ times the entropy production rate [see (4.6)–(4.8)]. Hence we define $T(x)$, for each configuration x, by $\sum_j(\mathbf{p}_j^2/2m)=Nj_B T(x)$ and [by (1.4)]

$$j_h\overset{\text{def}}{=}\frac{2N-1}{2N}\left\langle\frac{J_h}{k_B T}\right\rangle=\lim_{\tau\to\infty}\frac{1}{L^2}\frac{\sum_j\bar{\Lambda}_{u,\tau}^{-1}(x_j)\,\delta_\tau^{-1}(x_j)\,\partial_{E_h}\bar{\sigma}_\tau(x_j)}{\sum_j\bar{\Lambda}_{u,\tau}^{-1}(x_j)\,\delta_\tau^{-1}(x_j)} \tag{5.2}$$

where $\bar{\sigma}(x)=(1/\tau)\sum_{r=-\tau/2}^{\tau/2-1}\sigma(S^r x)$ [see (4.7)]. If we recall (4.3) with $\frac{1}{2}\tau=M$, we see that j_h can be regarded as the SRB average of $J_h/k_B T$, $h=1,2$.

This expression is similar to the formula derived from the generating function of the Helfand moments in refs. 27 and 28, but it is not the same because in ref. 28 the SRB is represented by using the noion of (ε,τ)-separated sets (which are a somewhat more primitive or less concrete version of the parallelograms of the Markov partitions).

We shall also define $l_{u,\tau}$, $l_{s,\tau}$ through

$$\bar{\Lambda}_{u,\tau}^{-1}(x)\,\delta_\tau^{-1}(x)=e^{\tau l_{u,\tau}(x)},\qquad \bar{\Lambda}_{s,\tau}(x)\,\delta_{-\tau}^{-1}(x)=e^{\tau l_{s,\tau}(x)} \tag{5.3}$$

so that (4.6) implies $l_{u,\tau}(x)-l_{s,\tau}(x)=t_0\bar{\sigma}_\tau(x)$. Hence we see that, if $\partial_k\equiv\partial_{E_k}$,

$$\partial_k j_h=\frac{1}{L^2}\frac{\sum_j\bar{\Lambda}_{u,\tau}^{-1}(x_j)\,\delta_\tau^{-1}(x_j)[\partial_{hk}\bar{\sigma}_\tau(x_j)+\tau\partial_k l_{u,\tau}(x_j)\,\partial_h\bar{\sigma}_\tau(x_j)]}{\sum_j\bar{\Lambda}_{u,\tau}^{-1}(x_j)\,\delta_\tau^{-1}(x_j)}$$

$$-\frac{1}{L^2}\frac{\sum_j\bar{\Lambda}_{u,\tau}^{-1}(x_j)\,\delta_\tau^{-1}(x_j)\,\tau\partial_k l_{u,\tau}(x_j)}{\sum_j\bar{\Lambda}_{u,\tau}^{-1}(x_j)\,\delta_\tau^{-}(x_j)}$$

$$\times \frac{\sum_j \bar{\Lambda}_{u,\tau}^{-1}(x_j)\, \delta_\tau^{\times 1}(x_j)\, \partial_h \bar{\sigma}_\tau(x_j)}{\sum_j \bar{\Lambda}_{u,\tau}^{-1}(x_j)\, \delta_\tau^{-1}(x_j)}$$

$$= \frac{1}{L^2} \langle \partial_{hk} \bar{\sigma}_\tau \rangle + \frac{\tau}{L^2} (\langle \partial_k l_{u,\tau} \partial_h \bar{\sigma}_\tau \rangle - \langle \partial_k l_{u,\tau} \rangle \langle \partial_h \bar{\sigma}_\tau \rangle) \tag{5.4}$$

Here we have interpreted the derivatives with respect to E_h of $\bar{\sigma}_\tau(x)$ and $l_{u,\tau}(x)$ by regarding x as $\mathbf{E}$ independent. However, this is *not* quite correct: in fact it is clear that we must consider such functions as defined on the attractor, not on the full phase space. The attractor depends on $\mathbf{E}$: it can in fact be identified with the unstable manifold W_O^u of a fixed point O or of a periodic orbit O (see ref. 25, Section 4): hence the point x_j, which has to be throught of as a point on the attractor, will change with $\mathbf{E}$ even though it keeps the same symbolic representation (note that the Markov partition changes with $\mathbf{E}$ although the compatibility matrix does not, by the structural stability theorem of Anosov,[11] at least if $\mathbf{E}$ is small).

In taking the derivatives with respect to $\mathbf{E}$ of $l_{u,\tau}(x_j)$ and in defining the current as $\partial_{E_h} \bar{\sigma}_\tau(x_j)$ there are therefore additional proportional to $\partial_{E_h} x$. The latter quantity can be considered as a function of the symbolic history of x, i.e., as the function $\partial_{E_h} x(\mathbf{j})$ and ref. 22 makes the following conjectured:

Conjecture. The function $\partial_{E_h} x(\mathbf{j})$ is a local function in the sense of the second theorem in Section 4 for all Anosov systems, or Axiom A systems, depending smoothly on parameters $\mathbf{E}$.

Assuming the validity of the conjecture and using it to perform rigorously an interchange of limits, one can check (see ref. 22 for details) that the extra terms in the $\mathbf{E}$ derivatives of $\bar{\sigma}_\tau(x(\mathbf{j}))$, $l_{u,\tau}(x(\mathbf{j}))$ at fixed history $\mathbf{j}$ just discussed *give no contribution* to the end result, i.e., they do not alter the validity of Onsager's reciprocity or of the fluctuation-dissipation relation derived below. Therefore, to avoid formal intricacies, we shall not take into account the extra terms and we proceed by ignoring them in (5.4) as well as in the following. The above conjecture has a mathematical nature and I do not discuss its proof here: I have not attempted to prove it (it seems closely related to Anosov's structural stability theorem[11]).

By using the time-reversal invariance we see that

$$\begin{aligned}\langle \partial_k l_{u,\tau} \partial_h \bar{\sigma}_\tau \rangle &= Z^{-1} \sum \bar{\Lambda}_{u,\tau}^{-1}(x_j)\, \delta_\tau^{-1}(x_j)\, \partial_k l_{u,\tau}(x_j)\, \partial_h \bar{\sigma}_\tau(x_j)\\ &= (2Z)^{-1} \sum_j (\bar{\Lambda}_{u,\tau}^{-1}(x_j)\, \delta_\tau^{-1}(x_j)\, \partial_k l_{u,\tau}(x_j)\, \partial_h \bar{\sigma}_\tau(x_j)\\ &\quad + \bar{\Lambda}_{u,\tau}^{-1}(ix_j)\, \delta_\tau^{-1}(ix_j)\, \partial_k l_{u,\tau}(ix_j)\, \partial_h \bar{\sigma}_\tau(ix_j))\end{aligned} \tag{5.5}$$

where Z denotes the "partition sum," i.e., the sum in the denominator of (5.4), and the averages are with respect to the distribution $\mu_{\tau/2,\tau}$.

Recalling that [see (4.5), (4.6), (5.3)] $l_{u,\tau}(ix)=l_{s,\tau}(x)$, $\bar{\sigma}_\tau(ix)=-\bar{\sigma}_\tau(x)$, we find that this becomes

$$(2Z)^{-1}\sum_j (\bar{\Lambda}_{u,\tau}^{-1}(x_j)\,\delta_\tau^{-1}(x_j)\,\partial_k l_{u,\tau}(x_j) - \bar{\Lambda}_{s,\tau}(x_j)\,\delta_{-\tau}^{-1}(x_j)\,\partial_k l_{s,\tau}(x_j))\,\partial_h\bar{\sigma}_\tau(x_j) \tag{5.6}$$

The derivatives at $E_1=E_2=0$ can be computed immediately by noting that *in such a case*, $\bar{\Lambda}_{u,\tau}(x)\,\bar{\Lambda}_{s,\tau}(x)\,\delta_\tau(x)/\delta_{-\tau}(x)\equiv 1$ [see (4.6)]. If we use that (4.6) implies $l_{u,\tau}-l_{s,\tau}=t_0\bar{\sigma}_\tau$, then it follows from (5.6) that [note that $\langle\partial_h\bar{\sigma}_\tau\rangle=0$ at $\mathbf{E}=\mathbf{0}$ by symmetry]

$$(\langle\partial_k l^{u,\tau}\partial_h\bar{\sigma}_\tau\rangle - \langle\partial_k l_{u,\tau}\rangle\langle\partial_h\bar{\sigma}_\tau\rangle)|_{\mathbf{E}=\mathbf{0}} = \frac{t_0}{2}\langle\partial_k\bar{\sigma}_\tau\partial_h\bar{\sigma}_\tau\rangle\Big|_{\mathbf{E}=\mathbf{0}} \tag{5.7}$$

We also see that (since also $\langle\partial_{hk}\bar{\sigma}_\tau\rangle$ vanishes in the present case)

$$\partial_k j_k|_{\mathbf{E}=\mathbf{0}} = \lim_{\tau\to\infty}\frac{t_0}{2\tau L^2}\sum_{m=-\tau/2}^{\tau/2-1}\sum_{n=-\tau/2}^{\tau/2-1}(\langle\partial_k\sigma(S^m\cdot)\,\partial_h\sigma(S^n\cdot)\rangle) \tag{5.8}$$

where the averages in the r.h.s. are with respect to $\mu_{\tau/2,\tau}$.

Hence we see that, apart from a further problem of interchange of limits (see below), (5.8) becomes

$$\partial_k j_h|_{\mathbf{E}=\mathbf{0}} = \frac{t_0}{2L^2}\sum_{m=-\infty}^{\infty}\langle\partial_k\sigma(S^m\cdot)\,\partial_h\sigma(\cdot)\rangle \tag{5.9}$$

where the averages are with respect to the SRB distribution (i.e., to the limit of $\mu_{\tau/2,\tau}$) at $\mathbf{E}=\mathbf{0}$.

The problem of interchange of limits is easily solved: under our assumption that the system is a transitive Anosov system the correlations of smooth observables decay exponentially (because they become local observables in the symbolic dynamics interpretation of the evolution provided by the Markov partitions), not only for μ, but also for $\mu_{\tau/2,\tau}$ (in the natural sense in which this may be interpreted in a finite-τ case; e.g., by regarding the interval $[-\tau/2, \tau/2]$ as a circle), and uniformly in τ.

The relation (5.9) implies that, setting $L_{hk}=\langle\partial_h j_k\rangle|_{\mathbf{E}=\mathbf{0}}$,

$$L_{hk}=L_{kh} \tag{5.10}$$

follows. Note that (5.9) expresses the *fluctuation-dissipation* relation relation between the transport matrix L and the current–current equilibrium correlation.

In the case of the model in Section 3 the situation is similar. If $\sum_{\mathbf{q}_j\in\mathscr{B}}\mathbf{p}_j^2/m=2Nk_{\mathrm{B}}T(x)$ and J_q denotes the heat $-q_+=-Q_+/L^2$ received by the gas from the thermostat $\mathscr{R}_+$ per unit time and volume, then

$$\begin{aligned}\frac{J}{k_{\mathrm{B}}T}&=\frac{(2N-1)}{L^2}\frac{\sum_{\mathbf{q}_j\in\mathscr{B}}\mathbf{p}_j\cdot\mathbf{i}/m}{\sum_{\mathbf{q}_j\in\mathscr{B}}\mathbf{p}_j^2/m}=\frac{1}{|\mathscr{B}|}\partial_E\sigma\\ \frac{1}{T_+}\frac{J_q}{k_{\mathrm{B}}T_+}&=\frac{2N_+-1}{|\mathscr{B}|}\frac{-Q_+}{2N_+k_{\mathrm{B}}T_+^2}=\frac{1}{L^2}\partial_{\delta T}\sigma\end{aligned}\tag{5.11}$$

Hence the above argument yields, for the model in Section 3,

$$\partial_{\delta T}\left\langle\frac{J}{k_{\mathrm{B}}T}\right\rangle\bigg|_{\delta T,E=0}=\partial_E\left\langle\frac{1}{T}\frac{J_q}{k_{\mathrm{B}}T}\right\rangle\bigg|_{\delta T,E=0}\tag{5.12}$$

In general we can consider changing the two parameters denoted a, b, the *thermodynamic forces*, which control the equations of motion of the system. Suppose that the entropy generation per unit time σ has the form

$$\sigma=\sum_r D_r\frac{Q_r}{\sum^r\mathbf{p}_j^2/m}\tag{5.13}$$

where $\sum^r$ denotes that the coordinates $\mathbf{q}_j$ are coodinates of a particle belonging to a group of N_r particles whose phase points are constrained by the rth constraint that we impose on the system (to fix the coordinates that would evolve with a zero Lyapunov exponent, in the thermodynamic limit). Let D_r be the number of degrees of freedom of the rth group of particles (in two space dimensions $D_r\simeq 2N_r$); then the above argument can be immediately generalized to yield that the *flows* $j_a=\langle\partial_a\sigma\rangle$ and $j_b=\langle\partial_b\sigma\rangle$ satisfy

$$\partial_b j_a|_{a,b=0}\stackrel{\text{def}}{=}L_{12}=L_{21}\stackrel{\text{def}}{=}\partial_a j_b|_{a,b=0}\tag{5.14}$$

which is a general Onsager reciprocity relation among "thermodynamic forces" and "currents." From (5.7) we also see that the matrix $\partial_b J_a$ is positive definite.

Note that, as mentioned above, in defining $\partial_a\sigma$, $\partial_b\sigma$ one has really to think of σ as defined on the space of the symbolic sequences $\sigma=\sigma(x(\mathbf{j}))$ [so that

$$\partial_a\sigma=\frac{\partial\sigma}{\partial a}(x(\mathbf{j}))+\frac{\partial\sigma}{\partial x}\frac{\partial x(\mathbf{j})}{\partial a}$$

this is conceptually different from the "naive" $(\partial\sigma/\partial a)(x(\mathbf{j}))$, although *in the above models* it does not affect the end reult: see Appendix B].

6. REMARKS

1. The models in Sections 2 and 3 have been considered as undergoing transformations at constant energy U. This is not very satisfactory, as one also, and mainly, wants to understand models in which the internal energy is allowed to change, at least when the model is such that in the absence of the constraint imposing constant U it still reaches a stationary state (i.e., if one can justify an *a priori* bound on the maximal kinetic energy that can attained before "dissipation" effects prevail).

According to the analysis of ref. 25, Section 8, and ref. 22, this case could still be treated by imposing that U is constant provided the constant value is fixed on the basis of what could be called a *dynamical equation of state* of the system. The latter is the relation linking the stationary average value of the energy U to the other system parameters

$$U = f(E^1, E^2), \qquad U = f(E, T_-, T_+) \tag{6.1}$$

in the cases of models like those in Sections 2 and 3 modified in order to (while keeping reversibility) admit *a priori* bounds sufficient to expect approach to stationarity as $t \to \infty$, even though the total energy is not conserved.[7] Here f should be determined by the dynamics itself, but its computation will require mathematical difficulties that we cannot expect to be able to solve (in general).

A similar analysis applies if one did wish to study the dynamics of the model in Section 2 with an *a priori* fixed total momentum in the horizontal direction: we expect that we can freely add to the equations of motion a minimal constraint force imposing the constraint $\mathbf{P} = P(E^1, E^2)\mathbf{i}$ if $P(E^1, E^2)$ is the average horizontal momentum in the stationary state, i.e., what could be called the (unknown) nonequilibrium "equation of state" of the system (and the implied $\dot{\mathbf{C}} = \text{const}$). This means that considering modified equations of motion

$$\dot{\mathbf{q}}_j = \frac{1}{m}\mathbf{p}_j, \qquad \dot{\mathbf{p}}_j = \mathbf{F}_j + E_j i - \alpha \mathbf{p}_j - \boldsymbol{\beta} \tag{6.2}$$

with the "multiplier" $\boldsymbol{\beta}$ given by $[(E_1 N_1 + E_2 N_2)/(N_1 + N_2)]\,\mathbf{i} - \alpha \mathbf{P}/(N_1 + N_2)$, should not lead to appreciably different qualitative behavior if the initial data are consistent with the equation of state $\mathbf{P} = P(E^1, E^2)\,\mathbf{i}$.

[7] If some simply suppresses the constraint that U is constant for the models of Sections 2 and 3, then it seems reasonable that the system does not approach a stationary state, not even when the forcing fields are small. Here f should be determined by the dynamics itself, but its computation will involve mathematical difficulties that we cannot expect to be able to solve (in general).

2. It is quite clear that the discussion of the previous sections can be extended to many other models. But it is not clear how far one can really extend the considerations. For instance, it would be desirable to extend, if possible, the considerations to a microscopic model of a macroscopic continuum obeying the macroscopic equations for a fluid or a mixture of fluids (possibly with chemical reactions allowed), as defined in ref. 9.

3. Onsager relations are often regarded as consequences solely of the reversibility of the equilibrium dynamics (see, however, ref. 29); one would therefore be led to infer that they *must* hold also for our models simply because they could be derived "as usual," and there would be no point in deriving them from the chaotic principle considerably weakening the strength of the interpretation of the present paper as a confirmation of the chaotic hypothesis.

Hence it is worth pointing out that the "usual derivation" rests on several assumptions, none of which is needed *if* the chaotic hypothesis is retained, at least in a dynamics of the type considered in the above models.

4. The "usual derivation" assumptions are the following:

(a) *Linear law*, i.e., the "time behavior of the state parameters can be described by linear equations" linking them to the driving forces; see ref. 9, pp. 36, 100.

(b) The "Boltzmann postulate": i.e., the entropy occurring in the macroscopic equations at a point ξ in space is proportional (via Boltzmann's constant) to the logarithm of the phase space volume (in the microcanonical equilibrium ensemble) of the microscopic states in which the state variables deviate from equilibrium by the amount they actually do at the point x (note that this is an assumption). Therefore the entropy is $-\frac{1}{2}(\mathbf{a}, G, \mathbf{a})$, quadratic in the deviations $\mathbf{a}$ from equilibrium; it has a maximum at zero deviations.

(c) The equilibrium evolution is *reversible.*

Then it follows that the time evolution of a fluctuation, i.e., a deviation from equilibrium of the order of the square root of the volume in which it occurs, is Gaussian [because of (b)]. This property is used to deduce [in combination with (c), (a)] that the "state parameters" $\mathbf{a}$, the flows $\mathbf{j}$, and the thermodynamic forces $\mathbf{X}$ satisfy $\dot{\mathbf{a}} = \mathbf{j} = L\mathbf{X}$ and the symmetry $L = L^T$; see ref. 9, pp. 101–102.

An initial (distribution of) microscopic configurations, close to the equilibrium state, generates a macroscopic state in which fluctuations are possible: so one can consider the free evolution of a state in which the initial "state parameters" have an average value off by the amount of a fluctuation size. The evolution will then satisfy the above "symmetry" relation.

For instance, $\mathbf{a} = (a_1, a_2)$ could be the horizontal center-of-mass coordinates of the two species of particles, in model 1 above, of a small volume around a point ξ.

The connection with "reality" requires further assumptions. Considering our model 1 for definiteness, suppose that we act on the system with small forces, thus driving an evolution of the average values of the "state parameters" $t \to \mathbf{a}(t)$ and creating an entropy per unit time $(\dot{a}_1 N_1 E^1 + \dot{a}_2 N_2 E^2)/T$ (see Section 2; this makes sense for small fields when the temperature T can be identified with the average kinetic energy per particle).

(d) Then Onsager supposes (see ref. 35: "As before we shall assume that the average regression of fluctuations obey the same laws as the corresponding macroscopic irreversible processes") that a fluctuation forced by external forces evolves as if it had occurred spontaneously by *regression law*, if $\mathbf{X}$ is given, $\mathbf{X} = (N_1 E^1, N_2 E^2)/T$, recalling that $N_1 = N_2 = N/2$, then $\dot{\mathbf{a}} = (N/2)\, L\mathbf{E}/T$ [or $\mathbf{j} = (N/2)\, L\mathbf{E}/T$, in the notations of the present paper], with $L_{12} = L_{21}$. Note that this is done (and can only be correct) up to corrections $O(\mathbf{E}^2)$, hence this famous hypothesis is often called the *linear regression law*.

Other derivations are more fundamental and are based on kinetic theory[5,9] or on the pure microscopic dynamics,[8,9] but still they rely on various assumptions besides time reversibility of the equilibrium dynamics: see ref. 43, pp. 85–96, for a modern discussion of the matter (in the form of an analysis of the Green–Kubo formulas).

5. With our chaotic hypothesis all the above assumptions (a)–(d) are *not necessary* if one considers the models in Sections 2 and 3 because the final result (i.e., $\mathbf{j}$ proportional to $L\mathbf{E}$ with L symmetric and positive definite) has been drawn without further hypotheses (other than the mathematical conjecture in Section 5). Of course, assuming the reversibility of the dynamics *even* in nonequilibrium (close to equilibrium) *and* the chaotic hypothesis is in some sense much stronger than the assumptions (a)–(d) [but note that the reversibility in nonequilibrium, close to equilibrium, is a form of assumption (c)]. It has, *however*, the basic advantage of being a conceptually simple general assumption for nonequilibrium statistical mechanics, which should furthermore be valid without even the restriction of being close to equilibrium.

One should add that, although reversibility of the nonequilibrium dynamics is assumed in this paper, it is quite likely that the ideas and methods can be extended to genuinely nonreversible models. Attempts at such applications can already be found in refs. 24, 25, and 22 and I hope that they can be generalized to more general physical situations quite beyong the, so far special, cases mentioned; see also ref. 29.

6. A much debated question is the extension of the Onsager relations to the really nonequilibrium regime (i.e., not close to equilibrium). In this case the very notion of reciprocity becomes ill defined. The chaotic hypothesis in principle applies also in the nonlinear regimes, but it is unlikely that it can be as powerful a tool to cover deterministic versions of the concrete, exactly treated, stochastic models of ref. 29.

7. A puzzling aspect of the chaotic hypothesis is that it implies that the system has a positive gap separating from zero the Lyapunov exponents, and one may have serious doubts (see refs. 34, 11, 14, and 17 on the validity of such a strong property, so that a discussion is in order.

This is taken up in ref. 25, Section 8, and ref. 22 by suggesting that there may well be many vanishing exponents [or exponents of $O(N^{-1})$ if N is the particle number]: such exponents should be "ignored," as they should correspond to macroscopic evolution laws which microscopically will be effectively described by local conservation laws.[15,31,33] They have an approximate character, unless $N \to \infty$, but one can think of imposing them as *exact* conservation rules by adding to the forces acting on the system other suitable "auxiliary" forces *minimally* required to achieve the purpose of turning the slow macroscopic observables responsible for the existence of the zero Lyapunov exponents into exact local conservation rules. For instance, one can find the auxiliary forces by applying the Gauss *principle of least constraint* (see Appendix A). The dynamical system obtained in this way should be one to which the chaotic hypothesis should apply, giving us hope that the analysis of the present paper might be generalizable to rather more general cases.[22]

8. A comment can be made at this point (at a referee's request) about the physical meaning of Gaussian thermostats. As suggested in refs. 18 and 19, one can expect that nonequilibrium stationary states are describable in several equivalent ways, as in the corresponding equilibrium cases many *ensembles* have the same physical content. Therefore Gaussian thermostats may be equivalent to other thermostats, with a more physical *look*. However, as argued also in remarks 1 and 7 above and in more detail in ref. 22, it seems clear that not all thermostats can be equivalent, as each thermostatting mechanism has a physical meaning and it may correspond to different stationary states. The antonym of "equilibrium" is "nonequilibrium," but the latter concept is much wider and it accommodates a larger variety of phenomena.

9. A referee remarks that it is, in fact, easy to generalize the above derivation of Onsager reciprocity to the case where the microscopic time reversal requires also the reversal of the applied fields a with some time parities ε_a. In that case, the so-called Onsager–Casimir relations (see ref. 9, Chapter VII, Section 4) are valid by the same proof.

APPENDIX A. THE GAUSS MINIMAL CONSTRAINT PRINCIPLE

Let $\varphi(\dot{\mathbf{x}}, \mathbf{x}) = 0$, $\mathbf{x} = \{\dot{\mathbf{x}}_j, \mathbf{x}_j\}$, be a constraint and let $\mathbf{R}(\dot{\mathbf{x}}, \mathbf{x})$ be the constraint reaction and $\mathbf{F}(\dot{\mathbf{x}}, \mathbf{x})$ the active force.

Consider all the possible accelerations **a** compatible with the constraints and a given initial state $\dot{\mathbf{x}}, \mathbf{x}$. Then **R** is *ideal* or *satisfies the principle of minimal constraint* if the actual accelerations $\mathbf{a}_i = (1/m_i)(\mathbf{F}_i + \mathbf{R}_i)$ minimize the *effort*

$$\sum_{i=1}^{N} \frac{1}{m_i} (\mathbf{F}_i - m_i \mathbf{a}_i)^2 \leftrightarrow \sum_{i=1}^{N} (\mathbf{F}_i - m_i \mathbf{a}_i) \cdot \delta \mathbf{a}_i = 0 \tag{A.1}$$

for all possible variations $\delta \mathbf{a}_i$ compatible with the constraint φ.

Since all possible accelerations following $\dot{\mathbf{x}}, \mathbf{x}$ are such that $\sum_{i=1}^{N} \partial_{\dot{\mathbf{x}}_i} \varphi(\dot{\mathbf{x}}, \mathbf{x}) \cdot \delta \mathbf{a}_i = 0$ we can write

$$\mathbf{F}_i - m_i \mathbf{a}_i - \alpha \partial_{\dot{\mathbf{x}}_i} \varphi(\dot{\mathbf{x}}, \mathbf{x}) = \mathbf{0} \tag{A.2}$$

with α such that $(d/dt)\, \varphi(\dot{\mathbf{x}}, \mathbf{x}) = 0$, i.e.,

$$\alpha = \frac{\sum_i (\dot{\mathbf{x}}_i \cdot \partial_{\mathbf{x}_i} \varphi + (1/m_i)\, \mathbf{F}_i \cdot \partial_{\dot{\mathbf{x}}_i} \varphi)}{\sum_i m_i^{-1} (\partial_{\dot{\mathbf{x}}_i} \varphi)^2} \tag{A.3}$$

which is the analytic expression of Gauss' principle.[32]

The Gaussian principle has been somewhat overlooked in the statistical mechanics literature: its importance has been only recently brought again to attention (see the review in ref. 30). A notable exception is a paper in which Gibbs[23] develops variational formulas which he relates to the Gauss principle of least constraint.

APPENDIX B. VANISHING OF THE CORRECTIONS TO (5.9)

This appendix refers to the last paragraph of Section 5. Starting from (5.2), it is appropriate, if one wants to keep track of the extra terms arising from the proper definition of $\partial_a \sigma$, to regard $\sigma(x)$ as a function $s(\mathbf{e}, x)$ of two arguments (thus making explicit mention of the $\mathbf{e}$ dependence of σ). Likewise the factors $l_{u,\tau}(x)$, $l_{s,\tau}(x)$ will be regarded as functions $\lambda_{u,\tau}(\mathbf{e}, x)$ and $\lambda_{s,\tau}(\mathbf{e}, x)$, etc. In this way the derivatives of $s(\mathbf{e}, \mathbf{x}_j)$ and $\lambda_{\cdot}(\mathbf{e}, x_j)$ can be easily followed.

The algebra of Section 5, performed without ignoring the $\mathbf{e}$ dependence of the points x_j, can be easily performed and it leads to some *extra terms* in (5.4). We write the result, for brevity, as follows:

$$\partial_k j_h|_{\mathbf{e}=\mathbf{0}} = (5.14) + \langle \partial_x s\, \partial_k x\, \partial_h s \rangle|_{\mathbf{e}=\mathbf{0}} + \langle \partial_{xk} s\, \partial_h x \rangle|_{\mathbf{e}=\mathbf{0}} \tag{B.1}$$

and the first correction term vanishes because $s(\mathbf{0}, \mathbf{x}) \equiv 0$, while the second extra term vanishes because

$$\langle \partial_{xk} s\, \partial_h x \rangle|_{\mathbf{e}=\mathbf{0}} = \partial_k \langle \partial_h s \rangle|_{\mathbf{e}=\mathbf{0}} - \langle \partial_h \partial_k s \rangle|_{\mathbf{e}=\mathbf{0}} \tag{B.2}$$

which is zero by time-reversal symmetry of the *equilibrium* ($\mathbf{e} = \mathbf{0}$) distribution.

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