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Lyapunov Instability of Classical Many-Body Systems

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Abstract. In this paper we are concerned with the instability of the phase-space trajectory for particle models resembling classical fluids with short-range interactions. Recently, the application of dynamical systems theory - and the computation of Lyapunov spectra in particular - has provided new and in some respect complementary insight both for systems in thermodynamic equilibrium and in nonequilibrium stationary states. Here, we summarize some of our work on this topic. In addition, taking stochastically-driven heat flows on planar lattices as an example, we discuss the existence and significance of fractal phase-space distributions for the understanding of such flows, independent of the driving mechanism.

1. Introduction

The Lyapunov instability of atomic or molecular systems is a consequence of the (basically) convex surface of the particles: An infinitesimal perturbation of the initial conditions is modified during each interaction event with neighboring particles and grows linearly with time in between. On average, this leads to exponential growth in time, which is characterized by a finite number of time-averaged rate constants, the Lyapunov exponents. The number of exponents is equal to the dimension, D, of phase space, and the whole set, $\{\lambda_1, \ldots, \lambda_D\}$, ordered according to size, $\lambda_l \geq \lambda_{l=1}$, is known as the Lyapunov spectrum. The numerical algorithms for continuous interaction potentials are generally based on the work of Benettin *et al.* [1] and Shimada and Nagashima [2] and require periodic re-orthonormalization of the associated perturbation vectors, $\delta_l(t), l = 1, \ldots, D$, with a Gram-Schmidt procedure. For methods with time-continuous re-orthonormalization we refer to the Refs. [3, 4]. For discontinuous potentials such as hard disks [5, 6] or hard dumbbells [7], the basic algorithm was derived by Dellago *et al.* [8]. It is important to note that for the ergodic systems we are concerned with in this paper, the Lyapunov exponents are properties averaged over the whole phase space and are independent of the initial conditions and of the metric. The instantaneous orthonormal perturbation vectors $\delta_l(t)$, however, are also independent of the initial conditions for large-enough t, but do depend on the metric in phase space.

2. Systems in thermodynamic equilibrium

The equations of motion for equilibrium Hamiltonian systems are generally symplectic and time reversible. This symmetry is also reflected in the Lyapunov spectrum: the exponents always appear in pairs, which sum to zero, $\lambda_l + \lambda_{D+1-l} = 0$. From a practical point of view this means that only positive exponents need to be computed. The vanishing of the sum of all exponents is a consequence of Liouville's theorem for the conservation of phase volume for symplectic systems. In the following we summarize results which were gained from a detailed analysis of the Lyapunov spectra for various systems:

1) For soft-potential fluids in two dimensions, the Kolmogorov-Sinai (or dynamical) entropy, h_{KS}, which is the rate with which information about the initial state of a system is obtained by subsequent measurements with a given accuracy [9], has a maximum at the fluid-to-solid phase transition [10, 11]. This means that the system is maximally chaotic at the transition point, and that all time scales characterized by the inverse Lyapunov exponents are involved in the rearrangement of the particles. Interestingly, if the density is varied at constant temperature, the maximum for λ_1, the maximum exponent, occurs for smaller densities than the maximum for the KS-entropy, which is the sum of all positive exponents. Thus, the Lyapunov spectrum provides novel and complementary information on phase transitions. For hard-particle fluids, however, no relative maximum for λ_1 or h_{KS} is observed, if the collision frequency is used as the order parameter instead of the density [8, 11].

2) Extensive simulations of hard dumbbell fluids [12, 13, 7] show that the translational and rotational degrees of freedom of linear molecules affect the Lyapunov spectrum in a very specific way. For molecular anisotropies below a certain density-dependent threshold, the translational part of the Lyapunov spectrum is effectively decoupled from the rotational part. For anisotropies above the threshold, there is mixing between rotational and translational degrees of freedom. Full roto–translational states may be expected only in this regime.

3) Since the *maximum (minimum)* Lyapunov exponent, λ_1 (λ_D) is the rate constant for the fastest growth (decay) of a phase-space perturbation, it is dominated by the fastest dynamical events, binary collisions in the case of a low-density gas. The associated perturbation vector has components which are strongly localized in physical space [14, 13]. Similar observations for other spatially-extended systems have been made [15, 16, 17, 18]. The particle-number dependence of the localization measure [7, 19] indicates that for both hard and soft disk systems the localization persists even in the thermodynamic limit, $N \to \infty$ [6, 11]. So far, no formal proof of this limit exists [20]. The localization becomes gradually less pronounced for larger Lyapunov indices $l > 1$ (smaller exponents), until it ceases to exist and (almost) all particles collectively contribute to the perturbations associated with the smallest Lyapunov exponents, for which coherent modes (see below) exist.

4) Even more exciting has been the recent discovery of Lyapunov modes. Lyapunov modes are periodic spatial patterns observed for the perturbations associated with the small positive and negative Lyapunov exponents. They are characterized by well defined wave vectors k,

$$k = \sqrt{\left(\frac{2\pi}{L_x} n_x\right)^2 + \left(\frac{2\pi}{L_y} n_y\right)^2} \;;\;\; n_x, n_y = 0, 1, \dots \;\;, \tag{1}$$

where a rectangular box with periodic boundaries is assumed, and where n_x and n_y denote the number of nodes parallel to x and y, respectively. Historically, Lyapunov modes were first observed for hard particle systems in one, two, and three dimensions [5, 21, 22, 19, 23], for hard planar dumbbells [12, 13, 7], for one-dimensional soft particles [24, 25], and, most recently, for soft-disk fluids [11]. For planar systems, their properties have been characterized in detail [22, 11]. Theoretically, they are interpreted as periodic modulations ($k \neq 0$) of the zero modes, to which they converge for $k \to 0$. Since a modulation, for $k > 0$, involves the breaking of a continuous symmetry (translational symmetry of the zero modes), they have been identified as Goldstone modes [26], analogous to the familiar hydrodynamic modes and phonons. The theoretical approaches for the computation of the Lyapunov exponents associated with modes have been based on random matrix theory [28, 29], periodic-orbit expansion [30], and, most successfully, kinetic theory [26, 31, 32]. Using kinetic theory and an expansion in k, de Wijn and van Beijeren succeeded in computing Lyapunov exponents to lowest order in the density and the wave vector [26]. Their results for the so-called transverse modes agree well with our computer-simulation results. The deviations for the so-called longitudinal modes, which still persist between the theoretical prediction and the simulations, are basically understood and may be improved [27].

3. Systems in nonequilibrium stationary states

Such systems are generated by the application of an external perturbation. The nature of this external perturbation is either mechanical (external fields, for example) or thermal (such as gradients of the volocity or temperature field). Since the perturbation does work on the system, which is dissipated into heat, a thermostating mechanism is required [33]. The thermostat(s) remove(s) the excess heat with a rate $\dot{Q}$. This is usually accomplished by a dynamical scheme, where a thermostat term with a thermostat variable ζ is added to the equations of motion, such that they *remain time-reversal invariant* [10, 34, 35, 36, 37]. The following important chain of thermodynamic relations holds [37]:

$$\left\langle \frac{d \ln \delta V}{dt} \right\rangle = -\frac{\dot{Q}}{k_B T} = -\left\langle \frac{d \ln f}{dt} \right\rangle = \frac{\dot{S}_G}{k_B} = -\frac{\dot{S}_{irr}}{k_B} = \sum_{l=1}^{D} \lambda_l = -\sum_i \langle \zeta \rangle < 0 \tag{2}$$

The first equality states that any infinitesimally-small phase volume, δV, co-moving with the phase flow, shrinks on average, which leads to an attractor and a fractal probability distribution, f, in phase space. As a low-dimensional illustration, we show in Fig. 1 the core of a multifractal

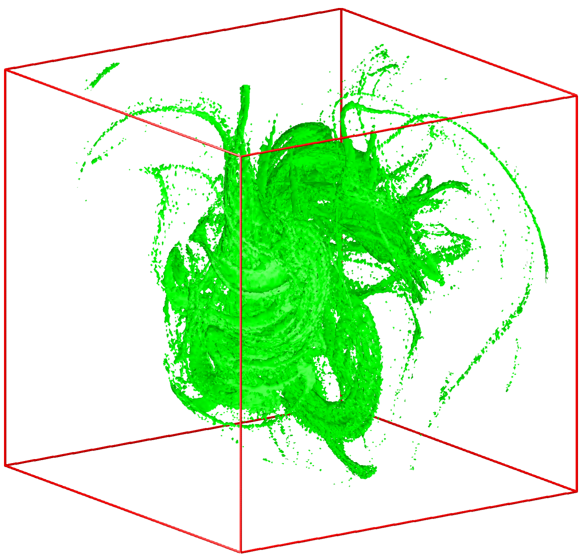

Figure 1. Attractor core for a one-dimensional oscillator model with heat conduction

attractor obtained from the Poincare map of a one-dimensional doubly-thermostated harmonic oscillator. The thermostat temperature varies with the coordinate q, such that for $q > 0$ the temperature is large and the oscillator gains energy from the thermostat, while for $q < 0$ the temperature is low and the oscillator loses energy. Thus, the oscillator conducts heat from the hot to the cold region [38, 39].

As a consequence of the phase-space collapse, the Gibbs entropy S_G diverges to $-\infty$ with time, wheras the rate of irreversible entropy production, $\dot{S}_{irr}$, is positive in the stationary state. In Eq. (2), k_B is Boltzmann's constant, and T is the *kinetic* temperature. Because $S_G \to -\infty$, the *thermodynamic* temperature, which is the derivative of the internal energy with respect to the entropy, is not defined for such nonequilibrium systems.

The collapse of the phase space measure leads to an information dimension D_1 smaller than the dimension of phase space, D, and may be determined from the Lyapunov spectrum. The sum of all exponents, $\sum_{l=1}^{D} \lambda_l$, is connected to the rate with which heat is flowing through the system and is, ultimately, extracted by the thermostat. As a consequence, $\langle \sum_i \zeta \rangle > 0$, where the sum is over all thermostated degrees of freedom. The last inequality assures that the transport coefficient associated with the external perturbation is always positive. The appearance of a fractal attractor, and the positivity of the transport coefficient, may be viewed as a consequence and fingerprint of the Second Law of thermodynamics. This is an important result. All these relations were found already in 1987 [40, 41], and were verified numerically for many systems [3, 42, 43, 44, 45, 4].

Theoretically, the existence of a fractal phase-space measure has also been proved for strictly hyperbolic systems (axiom-A systems), where it is referred to as Sinai-Ruelle-Bowen (SRB) measure [46]. A fractal probability distribution has been proved to exist for the driven Lorentz gas [47], although it is not strictly of this type. At present, the phase space collapse for many-body systems can be demonstrated only by computer simulation through the fact that the sum of all Lyapunov exponents becomes negative. This illustrates the significance of numerical studies of the Lyapunov spectrum for such systems.

Some physicists, however, are uneasy with time-reversible dynamical thermostats such as the Nosé–Hoover or Gauss thermostats [33]. Their usefulness for numerical computation is not disputed, but their physical significance is [52], since they cannot be constructed in the laboratory (unlike a block of copper). To consider this point in more detail, we recently constructed Lyapunov spectra also for a number of simplified systems which are thermostated by a *stochastic process* [49, 50, 54], for which random numbers are used for the generation of the phase trajectory. This construction assumes that the reference trajectory and all perturbed trajectories experience the same sequence of random numbers. In addition, it is explicitly assumed that the *first of the equalities* of Eq. (2) holds. The spectra obtained in this way could be shown to fulfill *all the equalities* and properties of Eq. (2) familiar from dynamical time-rversible thermostats.

Of course, this result is no proof for the real existence of fractal phase-space distributions for stochastically-driven stationary flows, i.e. systems with infinitely many degrees of freedom, since the connection between phase-space collapse and heat flow was explicitly put in. But it is an indication that Lyapunov spectra with properties intimately connected to the Second Law of thermodynamics may be constructed also in this case. It suggests that the precise nature of the thermostat - time-reversible or not–should be irrelevant. Starting from a completely different point of view, similar ideas were presented recently by D. Evans and collaborators [51], who argued that the precise nature of the thermostat should be irrelevant, if the interesting physical system is small (far fewer degrees of freedom) as compared to the thermostat. It would mean that the entropy production is a local property. We are still far from a rigorous proof of such an assertion.

Clearly, assertions of such fundamental significance need corroborative evidence. In the remainder of this paper we expand on the arguments given above by considering heat flow for a two-dimensional nonlinear lattice model.

4. Stochastically-driven heat flow on a planar nonlinear lattice

Recently, we studied heat flow in a square two-dimensional "ϕ^4" lattice model [4], where N particles are tethered with a *quartic* potential to the sites of a square lattice, and where nearest-neighbor particles interact with a *harmonic* potential. A stationary heat flow was maintained by two time-reversible Nosé–Hoover thermostats, one acting on the particle C in one corner and constraining it to a cold temperature T_C, the other acting on the particle H in the diagonally-opposite corner and keeping it at a hot temperature T_H. The full phase-space of this model has $4N + 2$ dimensions, where the 2 accounts for the time-reversible friction variables of the two thermostats. We found that the stationary heat flow is connected to a dimensionality loss, ΔD, of the phase-space density which may exceed the dimensionality associated with the directly-thermostated particles, $8 + 2$, by as much as a factor of four. As expected [53], ΔD turned out to be extensive in accord with irreversible thermodynamics. We estimated also the projection, $\Delta D_{\mathcal{H}}$, of the total dimensionality loss onto a subspace contributed by a number of non-thermostated, purely-Hamiltonian particles and found that nearly all of that loss occured in that subspace and persisted in the thermodynamic limit. This was a convincing example for the existence of a multifractal phase-space density for a stationary nonequilibrium system, for which almost-all degrees of freedom were not directly affected by a dynamical thermostat. However, the thermostats were time-reversible and subject to the criticism mentioned above.

Therefore, we consider here a stochastic version of this model, where the Nosé–Hoover thermostat for the hot particle is replaced by a *stochastic* thermostat, and where the fluctuating Nosé–Hoover friction variable is replaced by a *constant* friction coefficient. The energy, randomly injected by the stochastic force at a temperature T_H, is conducted through the system and is dissipated at a temperature $T_C < T_H$ by the constant friction of the cold particle. A stationary heat flow ensues, which is studied in the following.

We consider $N = 16$ particles on a 4×4 square grid with the cold particle located at the lower-left corner, $q_C \equiv q_1$, and the hot particle at the top-right, $q_H \equiv q_N$. The equations of motion are written as

$$\begin{array}{lllllllll} \dot{q}_H & = & p_H/m & ; & \dot{p}_H & = & F_H + A_H(t) & & \\ \dot{q}_i & = & p_i/m & ; & \dot{p}_i & = & F_i & ; & i = 2, \ldots, N-1 \\ \dot{q}_C & = & p_C/m & ; & \dot{p}_C & = & F_C - \zeta_C p_C, & & \end{array} \tag{3}$$

where p_H, p_i, p_C are the momenta of the hot, Newtonian, and cold particles, respectively. The forces F on the particles are derived from the quartic potential $(\kappa/4)\delta r^4$, tethering the particles to their lattice sites, and the harmonic nearest-neighbor potential $\phi(r) = \frac{\kappa_2}{2}(r-d)^2, r = |r_i - r_j| > 0$. The stochastic force $A_H(t)$ is assumed to be a δ-correlated random variable, for which

$$\langle A_H(0) \cdot A_H(t) \rangle = 4\zeta_H k_B T_H \delta(t), \tag{4}$$

and $\langle A_H^2 \rangle = 2\zeta_H k_B T_H$. As usual, k_B is the Boltzmann constant. The friction ζ_H, which controls the strength of the stochastic force, is related to the constant friction ζ_C of the cold particle according to

$$\zeta_H = \frac{T_C}{T_H} \zeta_C. \tag{5}$$

This ensures detailed balance and stationarity of the heat flow from the hot to the cold particle with kinetic temperatures $T_{H,C} = \langle p_{H,C}^2/2m \rangle$. If the stochastic force is averaged over one time step Δt,

$$\bar{A}_H \equiv \frac{1}{\Delta t} \int_t^{t+\Delta t} A_H(\tau) d\tau \equiv \{\bar{A}_\alpha\}$$

its components, $\bar{A}_\alpha, \alpha \in \{x, y\}$, are Gaussian random variables distributed according to the probability density

$$w(\bar{A}_\alpha) = (2\pi \langle \bar{A}_\alpha^2 \rangle)^{-1/2} \exp(-\bar{A}_\alpha^2 / 2\langle \bar{A}_\alpha^2 \rangle),$$

such that $\langle \bar{A}_\alpha \rangle = 0$, and $\langle \bar{A}^2_\alpha \rangle = 2m\zeta_H k T_H/\Delta t$. The momentum equation for the hot particle simply becomes

$$\dot{p}_H = F_H - \bar{A}_H. \tag{6}$$

The time-averaged rate of energy change,

$$\begin{aligned} \langle \dot{E} \rangle &= \frac{1}{m}\left[\langle p_H \cdot \bar{A}_H \rangle - 2\zeta_C k_B T_C \right] \\ &= \frac{1}{m}\left[\langle p_H \cdot \bar{A}_H \rangle - 2\zeta_H k_B T_H \right] = 0, \end{aligned}$$

vanishes in the stationary state, where the first term gives the rate of energy injected by the stochastic force, and the second the rate of energy dissipation by the cold-particle friction.

As mentioned before, the dynamics in tangent space is based on the *assumption* [50, 54] that the logarithmic rate of phase-volume change is determined by the heat flux, the first equality of Eq. (2). Subjecting the reference trajectory and the perturbed trajectories to the same sequence of random numbers, the linearized equations of motion become [4]

$$\begin{array}{lllllll} \dot{\delta q}_{H,\alpha} &=& \delta p_{H,\alpha}/m & ; & \dot{\delta p}_{H,\alpha} &=& \delta F_{H,\alpha} + A_H(t) \\ \dot{\delta q}_{i,\alpha} &=& \delta p_{i,\alpha}/m & ; & \dot{\delta p}_{i,\alpha} &=& \delta F_{i,\alpha} \qquad ; \quad i = 2, \ldots, N-1 \\ \dot{\delta q}_{C,\alpha} &=& \delta p_{C,\alpha}/m & ; & \dot{\delta p}_{C,\alpha} &=& \delta F_{C,\alpha} - \zeta_C \delta p_{C,\alpha}. \end{array} \tag{7}$$

Here, the force perturbation, $\delta F_i = \sum \frac{\partial F_i}{\partial q_j} \delta q_j$, for a particle i is a sum of contributions from all next-neighbor particles j. These equations provide the basis for our computation of the Lyapunov exponents for the stochastic ϕ^4 model. In the following we use reduced units, for which the particle mass m, the lattice constant d, the energy parameters κ and κ_2, and Boltzmann's constant k_B are unity.

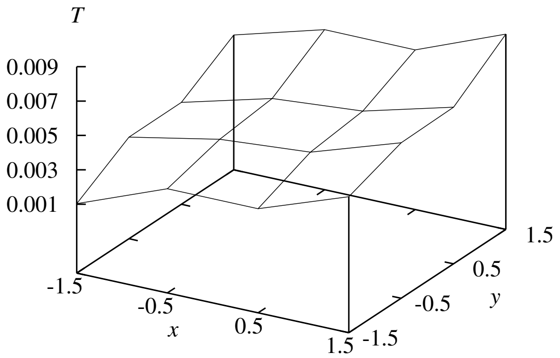

Figure 2. Temperature field for the driven stochastic 16-particle ϕ^4 model. $T_C = 0.001$, $\zeta_C = 0.5$, and $T_H = 0.009$, $\zeta_H = 0.056$.

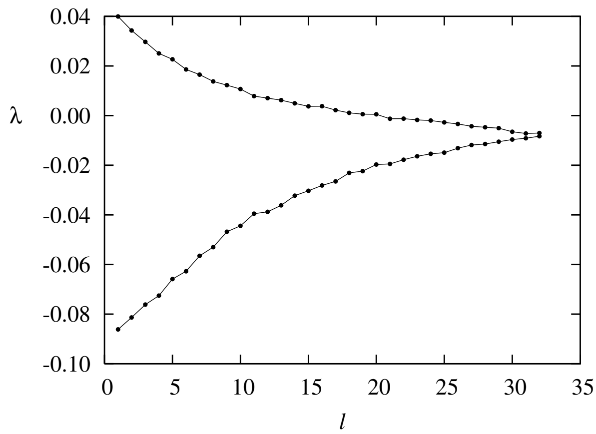

Figure 3. Lyapunov spectrum for the stochastic ϕ^4 model of Fig. 2.

The time-averaged temperature distribution is shown in Fig.2 for $T_C = 0.001$, $\zeta_C = 0.5$, and $T_H = 0.009$. These parameters are chosen so as to provide flows similar to the time-reversible

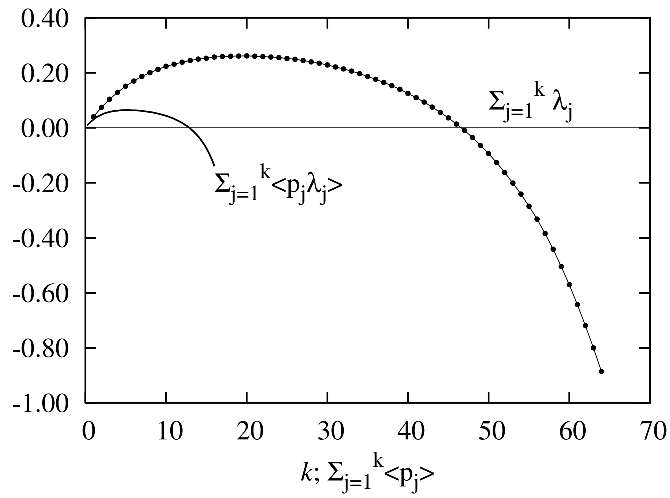

Figure 4. The points in the upper line denote the cumulative sum of Lyapunov exponents for the 16-particle ϕ^4 model in the full 64-dimensional phase space, leading to a Lyapunov dimension of 46.6 and, hence, a dimensionality reduction of 17.4. The lower line denotes the weighted exponent sums for the projection onto the 16-dimensional subspace of the four central particles and indicates a dimension of 12.8. Hence, the dimensionality reduction contributed by these four particles is 3.2.

case in Ref. [4]. One observes that the temperature profile is not linear, but this is not a serious limitation. Our main emphasis is on the dimensionality reduction ΔD of the phase-space density due to the flow, which is obtained from the Lyapunov spectrum, depicted in Fig. 3, by invoking the Kaplan-Yorke formula. From a plot of the cumulative sum of Lyapunov exponents, $\sum_{j=1}^{k} \lambda_j$, as function of $k,\ k = 1, \ldots, D$, in Fig. 4, we find $\Delta D = 17.4$. This number is comparable to the reduction previously found for the dynamically-thermostated model in Ref. [4].

With a method developed in Ref. [4], we estimate also the Lyapunov spectrum for the dynamics *projected* onto the 16-dimensional subspace of the four Newtonian particles in the center of the grid and compute the dimensionality loss $\Delta D_{\mathcal{H}}$ in this non-thermostated subspace of phase space. From the intersection of the lower line with the abscissa in Fig. 4 we deduce a dimension 12.8 for the projected distribution. Hence, the dimensionality reduction contributed by these particles is $16 - 12.8 = 3.2$. Although this number is considerably smaller than the projected reduction for the dynamically-thermostated case in Ref. [4], it is still significant.

5. Discussion

The fractal attractors one obtains in this way are indeed strange objects. They are referred to as "snapshot attractors" [55, 56] of a random dynamical system [57], and may be viewed as a blurred version of a strange attractor without randomness, where the fuzziness is generated by the random term appearing in the equations of motion. Due to this fuzziness, any stroboscopic map generates a smooth density of points in phase space, such that a simple box-counting method generates dimensions which agree with the dimensionality of phase space. We have verified this point by computing correlation dimensions D_2 both in the 16-dimensional subspace and the 8-dimensional configuration and momentum spaces of the four central particles of our model. If the correlation integral is computed from 200.000 points generated from the equations of motion (3) with a time spacing of 50 time units, we find about $D_2 \sim 15.5 \pm 0.5$ and $D_2 \approx 8$ for the respective cases. Since D_2 is strictly less or equal than D_1, the corresponding information dimensions are likely bigger than these numbers. However, the multifractal property of this random dynamical system is still derivable from the Lyapunov spectrum constructed in the way indicated above, which measures the local contraction rate at any instant of time.

Why do we look so hard for ways of constructing fractal phase-space probabilities for stationary nonequilibrium systems independent of the thermostating mechanism? Such strange attractors seem to be a very useful concept to understand the interplay between the microscopic dynamics and the Second Law for systems far from equilibrium. They could account for the irreversibility observed for such systems and would provide a connection to the observed transport properties. Evidence of their usefulness also comes from periodically perturbed systems. Already some time ago, we studied a very simple model, a periodically perturbed ensemble of uncoupled harmonic oscillators: It was shown that the states capable of sustaining a *perpetuum mobile* of the second kind are of measure zero and are fractally distributed on a Cantor-like set in phase space [58]. Thus, fractal sets seem to be a natural concept for interpreting the Second Law. Further theoretical work is needed to prove - or disprove - this idea.

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