Change in Distribution Function from Periodic Orbits

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Abstract

Using probability distributions obtained from periodic orbit expansions of steady states of thermostatted particle systems, we introduce a quantity which characterizes the distance of such steady states from equilibrium states. We call this property the periodic orbit entropy.

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1 Introduction

For an equilibrium ensemble of systems the Gibbs entropy is a well-defined and calculable property. In contrast, for a nonequilibrium ensemble of thermostatted systems, starting from an equilibrium initial state, the Gibbs entropy diverges with time towards minus infinity. Then, if an ensemble of systems initially at equilibrium is perturbed by an external field and a thermostat for a time T, and after that is left to relax by removing both the field and thermostat (i.e. it is left to relax by Hamiltonian evolution), the Gibbs entropy does not change from the value it had at T. If one believed that the Gibbs entropy represented the real entropy of the system, this would lead to the absurd result that the final entropy of the relaxed system depends upon the length of time T the field and thermostat were applied. Physically we expect that the

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nonequilibrium thermodynamic entropy can only depend on T if the system did not reach a steady state in that time. For all longer values of T, after the system has reached a steady state, we expect the relaxed system to have the same entropy regardless of the value of T. Moreover the Gibbs entropy for the relaxation to equilibrium remains constant rather than rising to the value of the equilibrium entropy. From this and other considerations, one concludes that the Gibbs entropy of thermostatted models cannot possibly represent the real entropy of the systems described by such models.

Despite this difficulty, various quantities related to the Gibbs entropy are currently used in the Statistical Mechanics literature in order to characterize nonequilibrium steady states of thermostatted systems, see, for instance [1,2]. Although it remains to be demonstrated that those quantities actually represent the thermodynamic entropy of nonequilibrium systems, we believe that they may be used to measure how far from equilibrium a system might be. In the same spirit, we use the idea of a periodic orbit measure to construct a particular kind of coarse grained Gibbs entropy, which measures the deviation of the phase space probability distribution of a nonequilibrium system in a steady state from its equilibrium counterpart. A similar approach has been used to calculate the configurational entropy of network-forming materials [3]. One could give a more detailed historical account of the well known debate on the use of the Gibbs and coarse grained Gibbs entropies in nonequilibrium statistical mechanics. However, we don't find this account particularly useful here, hence we refer the reader to the existing literature such as [1,2,4–7], where different views are presented.

As an example to illustrate what we have in mind, consider the field dependent thermostatted periodic Lorentz gas [8,9]. Although this example has only one moving particle our approach should be applicable to systems with more degrees of freedom, such as that in Ref [10]. The phase space for the thermostatted Lorentz gas is three dimensional as the constraint of constant kinetic energy eliminates one degree of freedom. One of these dimensions can be eliminated by taking as a Poincaré section the points of phase space corresponding to collisions of the moving particle with the surface of the circular scatterers (of radius $r = 1$). This way, a point on the Poincaré section is specified by the two angles (θ, ϕ) representing the direction of the velocity of the moving particle and the point of impact on the scatterers surface, respectively [9]. A periodic orbit representation of the steady state probability distribution in this two dimensional phase space can be constructed by searching for periodic points in the Poincaré section as done, for instance in [9]. In this context, exploiting the periodicity of the system, it suffices to consider the probability distribution in the elementary cell whose replicas tile the whole phase space. Then, there are two kinds of orbits that contribute to the probability distribution in phase space: those that are really periodic, and those that appear to be periodic in the elementary cell, being periodic only up to translation by an integer number of lattice vectors [11,12,6,13].

2 Periodic Orbit Measures

In the present paper we make one assumption which is empirically motivated by numerical results such as those of Refs [9,12,13]: we assume that periodic orbit (PO) expansions can be used to compute the averages of phase variables for the periodic Lorentz gas. In particular, let ω be an unstable periodic orbit of period τ_ω in the attractor Ω of the system, and let the quantity B_ω be defined by:

$$B_\omega = \frac{1}{\tau_\omega} \int_0^{\tau_\omega} B(S^t \Gamma_\omega) dt \tag{1}$$

where B is a function of phase, the integral is carried over one period of ω, and $S^t\Gamma_\omega$ is the point representing the state of the system at time t, if it was $\Gamma_\omega \in \omega$ at $t = 0$. Then, our assumption is the following.

Assumption: *Consider the dynamical system describing the Lorentz gas subjected to an electric field $\epsilon \geq 0$, and to a Gaussian thermostat. There is an invariant measure μ_ϵ such that*

$$< B >_\epsilon \equiv \lim_{T\to\infty} \frac{1}{T} \int_0^T B(S^t\Gamma) dt = \int_\Omega B(\Gamma_0) \mu_\epsilon(d\Gamma_0) \tag{2}$$

for (Lebesgue) almost all $\Gamma \in \Omega$. Moreover, the following periodic orbit expansion holds:

$$< B >_\epsilon = \lim_{\tau\to\infty} \frac{\sum_{\omega\in P_{\tau,\delta}(\epsilon)} \tau_\omega \Lambda_{\omega,u}^{-1} B_\omega}{\sum_{\omega\in P_{\tau,\delta}(\epsilon)} \tau_\omega \Lambda_{\omega,u}^{-1}}, \tag{3}$$

where $\Lambda_{\omega,u}$ is the Jacobian of S^{τ_ω} restricted to the unstable manifold of ω, B_ω is the average of B over ω and $P_{\tau,\delta}(\epsilon)$ is the set of unstable periodic orbits of period within $[\tau, \tau + \delta)$ for any $\delta > 0$, in the presence of the external field ϵ.

Equation (3), with B in the class of continuously differentiable functions, was proved in Ref [14] to hold for axiom-A flows, and expresses the average of B as a limit of weighted averages of orbital averages, where the weights have the suggestive form

$$\tau_\omega \Lambda_{\omega,u}^{-1} = (\textit{time spent in } \omega) \times (\textit{inverse instability of } \omega)$$

which attributes a higher weight to longer orbits with same instability, and a lower weight to more unstable orbits of same period. In this sense, the quantities $\tau_\omega \Lambda_{\omega,u}^{-1}$ can be used to define a probability density in phase space, which could be used to define a sort of coarse grained Gibbs entropy for the system under consideration. To do that, given any set $P_{\tau,\delta}(\epsilon)$ of finite period orbits, let us imagine that the dynamics has been reduced to a Poincaré section (which we also call Ω), and that this section can be partitioned into cells each characterized by a constant probability density. We then take this constant to be equal to zero if the cell contains no periodic points, and to be proportional to $\tau_\omega \Lambda_{\omega,u}^{-1}$, if the cell contains one point of the orbit ω. Because the periodic orbits in $P_{\tau,\delta}(\epsilon)$ are at most a finite number for any $\tau, \delta > 0$, one can always find a partition of Ω whose cells contain at most one periodic point. We assume that in our construction the number n_ω will be the number of collisions which the moving particle of the Lorentz gas undergoes along the orbit ω, and similarly to [9,12,13], we will group orbits with same n_ω, to form $P_{\tau,\delta}(\epsilon) = P_n(\epsilon)$, the set of unstable periodic orbits with n collisions. This way, at any finite n one obtains a non-singular probability distribution in Ω, of the following form:

$$\begin{aligned} f_\epsilon^{(n)}(\Gamma) &= \frac{\sum_{\omega \in P_n(\epsilon)} \Lambda_{\omega,u}^{-1} \tau_\omega \chi_\omega(\Gamma)}{\sum_{\omega' \in P_n(\epsilon)} \Lambda_{\omega',u}^{-1} \tau_{\omega'} V_{\omega'}} \\ &= \frac{1}{Z_\epsilon^{(n)}} \sum_{\omega \in P_n(\epsilon)} \Lambda_{\omega,u}^{-1} \tau_\omega \chi_\omega(\Gamma) \end{aligned} \tag{4}$$

where $\chi_\omega(\Gamma)$ is the characteristic function of the union of the n cells containing the n periodic points of orbit ω, i.e. is one if Γ is in that set and zero otherwise, and V_ω is the area of that set.

3 The Gibbs Entropy

The Gibbs entropy of the state represented by a measure μ_ϵ with a density f_ϵ, where ϵ is a parameter characterizing the dynamics, is given by

$$S_\epsilon = -\int d\Gamma f_\epsilon(\Gamma) \log f_\epsilon(\Gamma). \tag{5}$$

In the case that both μ_ϵ and μ_0 have densities f_ϵ and f_0, the change in Gibbs entropy between a state with $\epsilon = 0$ and a state with parameter ϵ would be given by

$$\Delta S_\epsilon = -\int d\Gamma f_\epsilon \log f_\epsilon + k \int d\Gamma f_0 \log f_0 . \tag{6}$$

Unfortunately, this is not the case for the thermostatted Lorentz gas [15] if ϵ represents the external field acting on the moving particles, and μ_ϵ is the corresponding natural measure. In fact, the dynamics of such a system is dissipative, and its natural measure is singular for all $\epsilon > 0$, hence Eq. (5, 6) do not make any sense in that context. Nevertheless, using the procedure outlined in the previous section, one can consider approximate probability distribution functions, which are not singular, by partitioning the phase space into cells each containing one periodic point [11,16]. One can then ask what are the changes undergone by these approximate probability distributions, as the external field changes from 0 to $\epsilon > 0$. For orbits of length n, these changes are reflected in the quantity:

$$\Delta S_\epsilon^{(n)} = -\int d\Gamma f_\epsilon^{(n)} \log f_\epsilon^{(n)} + \int d\Gamma f_0^{(n)} \log f_0^{(n)} \tag{7}$$

where each term on the right hand side will be called the n^{th} PO-entropy at the corresponding field (ϵ or 0 respectively). This may help to characterize in a more physically interesting fashion the changes undergone by the natural measure. In fact, it has been observed in [17–19], among others, that the phase space distribution function of the thermostatted Lorentz gas does not appear very different from the equilibrium uniform distribution, up to relatively high fields (of order $O(1)$), despite the fact that such a distribution is singular for all $\epsilon > 0$ (see, e.g., [20] for more general systems than ours). These apparently contrasting facts can be reconciled considering that the singularity of μ_ϵ for small ϵ manifests itself only on scales which cannot be easily observed. Indeed, in periodic orbit expansions such as Eq.(3), increasing the periods of the orbits corresponds to better and better approximations of the real averages $< B >_\epsilon$, but in practice orbits of relatively short period (orbits with $10 - 12$ collisions, in the Lorentz gas) afford a good representation of the steady states, for what concerns the most important physical observables, like the conductivity, the pressure, the Lyapunov exponents, etc [9,12,13]. Therefore, rather than looking at the change undergone by the real distribution, which collapses from uniform to singular as soon as the external field is made nonvanishing, it may be more interesting to look at the changes undergone by the approximate probability distributions constructed as in Sect 2, which are effectively used in the calculations of the physical observables.

ϵ	orbits	$\Delta\log(Z_\epsilon^{(4)})$	$\Delta S_\epsilon^{(4)}$
0.000	108	0.0000	0.0
0.001	99	-0.0156	-0.0103
0.005	90	-0.0370	-0.0905
0.010	84	-0.0457	-0.1226
0.100	73	-0.1777	-0.2388

Table 1
Variation of the PO properties with the field ϵ for PO's of 4 collisions. Here 'orbits' is the number of different periodic orbits of length 4, $\Delta\log(Z_\epsilon^{(4)})$ is the change in the logarithm of the PO partition function, and $\Delta S_\epsilon^{(4)}$ the total change in the PO-entropy from all terms on the right-hand side of equation (8).

4 Changes in the Approximate Distributions

For the Lorentz gas the total (or internal) energy consists of only the kinetic energy, which is constant, so the appropriate ensemble in this case is the microcanonical one, the uniform distribution in the usual billiard coordinates $(\phi, sin(\theta-\phi))$. Using the distribution in Eq. (4), one obtains

$$\Delta S_\epsilon^{(n)} = \log\left(\frac{Z_\epsilon^{(n)}}{Z_0^{(n)}}\right) - \sum_{\omega\in P_n(\epsilon)} \frac{\Lambda_{\omega,u}^{-1}\tau_\omega V_\omega}{Z_\epsilon^{(n)}} \log(\Lambda_{\omega,u}^{-1}\tau_\omega) + \sum_{\omega\in P_n(0)} \frac{\Lambda_{\omega,u}^{-1}\tau_\omega V_\omega}{Z_0^{(n)}} \log(\Lambda_{\omega,u}^{-1}\tau_\omega) \qquad (8)$$

The expression in equation (8) gives the change in the n^{th} PO-entropy (obtained from orbits containing a fixed number of collisions, n) which can also be taken as a measure of the variation in $f^{(n)}$ when the external field is changed from 0 to $\epsilon > 0$.

5 Numerical Results

A detailed study of the periodic orbits of the Lorentz gas in an applied field has been carried out by Lloyd et. al. [9,22]. As an initial feasibility calculation, we consider orbits of length 4 as these provide a reasonable sampling of the attractor. We calculate the contributions to various terms in equation (8), the first involving changes in the partition function $Z_\epsilon^{(4)}$ [21] alone and the others reflecting changes due to the change in the dynamical weights $\tau\Lambda_{\omega,u}^{-1}$ with field. The results are given in the following table (1).

The first noticeable effect is that the total number of periodic orbits decreases as the field increases. This decrease in orbits is due to pruning as the effect of an increase in the field changes the path of the periodic orbit and leads to intersections with scatterers (and hence removal of the orbit from the observable set). However, this is not the only effect as the change in orbit path may also allow new periodic orbits to arise. For example, for $N = 4$ and $\epsilon = 0.1$ there are 4 new orbits (in the 73) that do not appear at any other values of field considered here. The overall effect is still a net loss of orbits with increasing field. If we consider orbits of length 2 or 3 then the pruning as a function of field is more dramatic with typically half of the orbits lost at one change in field value. For $N = 4$ this pruning is more gradual, but the total number of orbits is not so large as to require large amounts of computer time to sample them accurately. For longer periodic orbits the sampling problems were such that comparison between different fields was no longer satisfactory with the available numerical data. ¿From equation (8) it is clear that the second and third terms on the right-hand side are nearly equal and opposite in sign. Therefore it is vital that the weights $\Lambda_{\omega,u}^{-1}(\epsilon)$ and the periods $\tau_\omega(\epsilon))$ are sufficiently accurate to make the results meaningful. To that end much more accurate numerical work has begun to check the accuracy of the present results and to extend the calculations to longer orbits to explore the convergence of the PO-entropy. These results will be reported separately. It is anticipated that the PO-entropy may initially appear to converge to a limit as the length of the orbit increases, but eventually diverge as finer and finer length scales are probed. However, the exponential proliferation of orbits may also lead to an apparent divergence, but importantly this problem will be the same for equilibrium as it is for nonequilibrium, so it is not the effect of a non-zero value of the field.

We conclude by observing that $\Delta S_\epsilon^{(4)}$ is monotonically decreasing with the field, like $\Delta \log(Z_\epsilon^{(4)})$ is. This indicates that both quantities $\Delta S_\epsilon^{(4)}$ and $\Delta \log(Z_\epsilon^{(4)})$ could be taken as measures of the distance of a nonequilibrium steady state from the corresponding equilibrium state.

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