

A Dynamical Partition Function for the Lorentz Gas

Gary P. Morriss,¹ Lamberto Rondoni,¹ and E. G. D. Cohen²

Received August 2, 1994; final December 30, 1994

In this paper we introduce a dynamically defined partition function for the Lorentz gas and investigate its connection with the classical ensembles and the phase-space probability measure derived from periodic orbit expansions. Numerical evidence is presented to support the equivalence of these measures and to link them to the thermodynamic quantities for the Lorentz gas. This also suggests a new dynamical basis for the assumption of equal *a priori* probabilities in the microcanonical ensemble.

KEY WORDS: Ensembles; periodic orbit expansion; singular orbital measures.

1. INTRODUCTION

The complete framework of classical statistical mechanics can be based on two postulates.⁽¹⁾ The first postulate is that of equal *a priori* probabilities for the distribution of ensemble members on the surface of constant energy, where each ensemble member is an isolated system with the same number of particles N , volume V , and energy E . This postulate implies that the *microcanonical ensemble* has a distribution given by

$$d\mu_{\text{mc}}(\Gamma) = \frac{\delta(H-E) d\Gamma}{\int \delta(H-E) d\Gamma} = \frac{\delta(H-E) d\Gamma}{S(E)} \quad (1)$$

where $S(E)$ is the area of energy surface $H(\Gamma) \equiv H(\mathbf{q}, \mathbf{p}) = E$. This is the probability that the system will be found inside a phase-space volume element $d\Gamma$, centered around $\Gamma \equiv (\mathbf{q}, \mathbf{p})$. It is much more usual to find that a system is not isolated, and the generic situation is to consider an equilibrium system in contact with a reservoir. If that reservoir is very large in comparison with the system of interest, then the system and reservoir will

¹ School of Physics, University of New South Wales, Sydney 2052, Australia.

² The Rockefeller University, New York, New York 10021-6399.

be in thermal equilibrium at the temperature of the reservoir (which is determined by its energy). An ensemble of such systems, each in contact with a reservoir at the same temperature, constitute the *canonical ensemble*.⁽¹⁾ The form of the phase-space distribution function for a canonical ensemble of systems can be a second postulate

$$d\mu_c(\Gamma) = \frac{e^{-H(\Gamma)/kT} d\Gamma}{\int e^{-H(\Gamma)/kT} d\Gamma} \quad (2)$$

Equation (2) defines what we will refer to as the canonical measure, where k is Boltzmann's constant. The denominator is known as the canonical partition function, $Z_c(N, V, T)$. The partition function normalizes the measure on the whole phase-space, thus making the canonical ensemble a probability measure, where $d\mu_c$ is the probability associated with the volume element $d\Gamma$. The logarithm of the partition function generates the thermodynamic properties of the system; in particular, the pressure is given by the following relation:

$$p = kT \frac{\partial}{\partial V} \ln Z_c(N, V, T) \quad (3)$$

In this paper we introduce a dynamical partition function for the Lorentz gas⁽²⁾ and propose a new dynamical basis for the microcanonical ensemble. The Lorentz gas considered in this paper has a point particle moving through a regular triangular array of stationary, hard-disk scatterers. The volume is changed by changing the interscatterer distance w , thus preserving the shape of the regular triangular lattice.

2. THE DYNAMICAL PARTITION FUNCTION

In recent years a number of works have been devoted to the study of the properties of chaotic systems in terms of the unstable periodic orbits (UPOs). These studies show that the natural measure for certain hyperbolic systems can be hierarchically approximated through measures supported on sets of progressively longer and longer unstable periodic orbits.⁽²⁻⁹⁾ In this approach, the UPOs are grouped into prime sets according to length, and measures of larger and larger support are constructed by assigning weights to each UPO. The (weak) limit of these measures can be proved to be the natural measure for Axiom A flows.⁽³⁾ The Lorentz gas has been studied using these methods, and although there is no proof of the validity of the UPO measures in this case, the accumulated evidence supports this approach.^(2, 4, 5)

The ideas involved in the periodic orbit expansion for the Lorentz gas can be illustrated physically as follows. Consider a probability measure

with support on the set of periodic orbits with n collisions (n fixed), and call it $\rho^{(n)}$. Clearly, from a dynamical point of view, $\rho^{(n)}$ must assign the same weight to each point $\Gamma = (\mathbf{q}, \mathbf{p})$ on a given UPO, and the chosen weight is proportional to the stability of the orbit. Indeed, regions close to less unstable orbits are visited by a generic chaotic trajectory more often than regions around more unstable periodic orbits, which results in a higher value of the natural measure in the regions around the less unstable orbits than around the more unstable ones. At the same time, for UPOs of equal stability, the larger their length, the easier it is to find them in phase-space. Thus, the weight assigned to UPOs is proportional to their length. As the stability of a UPO is measured by the inverse of its Lyapunov number, A_i , then the value of the measure for an element of phase-space around the point Γ in the orbit i of length n is

$$d\rho_{i \in P_n}(\Gamma) = CA_i^{-1} dl_i(\Gamma) \quad (4)$$

where P_n is the set of UPOs of length n ; C is a normalization constant independent of i ; and $dl_i(\Gamma)$ is the mass contributed by the uniform (orbital) measure supported on the UPO i to a given phase-space element.⁽³⁾ In other words, dl_i is a measure which gives zero weight to all the subsets of the phase-space which do not contain points on the UPO i , and it uniformly distributes the weight for all the points of i . Thus, $dl_i(\Gamma)$ is the length of the UPO segment inside $d\mathbf{q}$ (centered at \mathbf{q}), and the integral of $dl_i(\Gamma)$ over the whole phase-space is the spatial length of i . Given an arbitrary phase variable B , its average with respect to $d\rho_i$ can be written as

$$\langle B \rangle_{i \in P_n} = \int_{\text{Phase Space}} B(\Gamma) d\rho_i(\Gamma) = C(A_i)^{-1} \int_{\Gamma \in i} B(\Gamma) dl_i(\Gamma) \quad (5)$$

Note that, since the speed of the wandering particle in the Lorentz gas is one, a trajectory can be parametrized either in terms of its length or period. Generally, it is the time variable that is adopted in the literature. Using this notation, the average of B over all UPOs of length n is

$$\langle B \rangle_n = \left[\sum_{i \in P_n} A_i^{-1} \int_0^{\tau_i} B(\Gamma(t)) dt \right] / \sum_{i \in P_n} \tau_i A_i^{-1} \quad (6)$$

where τ_i is the period of orbit i . Here, Γ is a point on the phase-space trajectory of UPO, and it is considered as a function of the time which parametrizes the orbit. Correspondingly, the explicit expression of the measure with support on all the orbits of length n is

$$d\rho^{(n)}(\Gamma) = C \sum_{i \in P_n} A_i^{-1} dl_i(\Gamma) = \frac{A^{(n)-1}(\Gamma) d\tau^{(n)}(\Gamma)}{\sum_{i \in P_n} \tau_i A_i^{-1}} \quad (7)$$

where $A^{(n)-1}(\Gamma) = A_i^{-1}$ if $\Gamma \in i$, and $A^{(n)-1}(\Gamma) = 0$ otherwise; and $d\tau^{(n)}$ is the time needed by a particle on a UPO of length n to cross the space element dq around the space component of Γ . Note that, given a point on a UPO of length n , it is always possible to find a neighborhood of that point which does not contain any point from a different UPO of the same length. At all finite n , this allows us to construct nonoverlapping neighborhoods of the periodic orbits such that the fraction of phase-space they cover is arbitrarily small and positive, and to thereby assign a density to our orbital measures. Taking the limit $n \rightarrow \infty$ of these measures means taking the limit in the appropriate weak topology.

The theory of periodic orbit expansions states that the average of a phase variable according to the natural measure of the dynamics can be obtained by taking the $n \rightarrow \infty$ limit in Eq. (6). This procedure has been carried out for the pressure⁽²⁾ and the results obtained suggest that the UPO average is in excellent agreement with the time average. In Fig. 1 we compare our UPO average with the time average for different values of the spacing w . Invoking the ergodic theorem for this system,⁽¹⁰⁾ this implies that the UPO average agrees with the microcanonical ensemble average. This agreement holds for averages of other dynamical variables, such as the diffusion coefficient and the average Lyapunov exponent.⁽²⁾ Henceforth, we assume that this agreement holds for all phase variables B . Thus, if the limit $d\mu_d(\Gamma) = d\rho^{(\infty)}$ of the measures $d\rho^{(n)}$ exists, we can take it as the phase-space distribution function for the system. This constitutes a first example of the connection between the thermodynamic formalism of Ruelle⁽¹¹⁾ (which gives rise to the UPO expansion) and real thermodynamics.

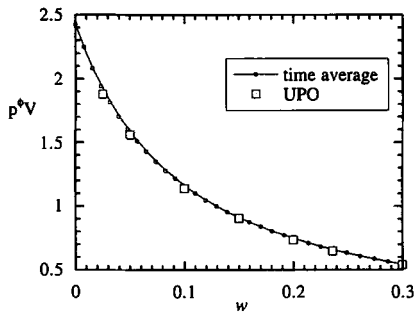


Fig. 1. Potential pressure times volume versus interdisk spacing w . The dots, fitted with a continuous curve, represent the results of direct simulations of around 10^6 collisions. The large squares represent the results obtained from the use of UPO measures, as computed for UPOs up to length 12.

We further argue that the normalization factor of the limiting UPO measure, which we term the *dynamical partition function*, is equivalent to the canonical partition function. That is, we define

$$Z_d(V) = \lim_{n \rightarrow \infty} Z^{(n)}(V) = \lim_{n \rightarrow \infty} \sum_{i \in P_n} \tau_i \exp(-\tau_i \lambda_i) \quad (8)$$

We observe that this partition function has the dimensions of time. This is analogous to the classical partition function for an N -particle system which has the units of action to the N th power. Before we take the logarithm we must make $Z_d(V)$ dimensionless by dividing by a characteristic time t_c . The value of this characteristic time only affects thermodynamic functions by at most a constant, as the t_c disappears in the difference between logarithms and when partial derivatives are taken. For the dynamical partition function to have physical meaning it must generate the thermodynamic properties of the system. We now construct a numerical test of this conjecture.

3. A NUMERICAL TEST OF THE DYNAMICAL PARTITION FUNCTION

The system that we use to study our hypothesis is the Lorentz gas, as in Section 2. This system is composed of an infinite array of hard scatterers (arranged on the sites of a triangular lattice in two dimensions) with a single point particle *wandering* through the lattice. This wandering particle experiences simple hard-core collisions with the scatterers. To construct a thermodynamics for this system we must first establish the microscopic representations for the macroscopic variables, temperature and pressure, and we do this starting from the general setting of interacting N -particles systems.

Consider the temperature of an equilibrium system of N particles in a d -dimensional space. Here the temperature is related to its kinetic energy by the equipartition theorem, which states that the average kinetic energy per degree of freedom equals $kT/2$. The total momentum of the system is usually constant in time (and vanishing), and the kinetic energy is also fixed. Therefore, the number of degrees of freedom of such a system reduces to $dN - d - 1$. Note that in the limit of large N , the quantity $(d + 1)$ is negligible, but for small N , such as the Lorentz gas, the correct counting of the number of degrees of freedom is crucial. It follows that the total translational kinetic energy is given by

$$K = \sum_{i=1}^N \frac{1}{2m} p_i^2 = (dN - d - 1) \frac{kT}{2} \quad (9)$$

where m is the mass of each particle, and p_i is the momentum of the i th particle. From linear response theory⁽¹²⁾ it can be shown that the pressure is given by

$$dpV = \frac{dN - d}{dN - d - 1} \sum_{i=1}^N \frac{1}{m} p_i^2 - \sum_{i < j} \mathbf{r}_{ij} \cdot \mathbf{F}_{ij} \quad (10)$$

where \mathbf{r}_{ij} is the vector joining particle i to particle j , and \mathbf{F}_{ij} is the force that particle i exerts on particle j . Combining Eqs. (9) and (10) gives

$$pV = (N - 1)kT - \frac{1}{d} \sum_{i < j} \mathbf{r}_{ij} \cdot \mathbf{F}_{ij} = (N - 1)kT + p^\phi V \quad (11)$$

Here, the pressure of the system has been decomposed into its kinetic contribution $(N - 1)kT/V$ and its potential (or interaction) contribution, which is given by p^ϕ . This reduces to the correct ideal-gas law with the usual N replaced by $N - 1$. It is clear that for large N there is no difference, but for a small system where, for example, $N = 2$, the correction plays an important role. We can map the $N = 2$ system described above onto the Lorentz gas by moving the coordinate origin from the center of mass of the system to the center of particle 1 and scaling the mass to ensure that the kinetic energy is invariant. Choosing the mass $M = 1$ and constant speed $p = 1^{(2)}$ for the wandering particle in the Lorentz gas gives $kT = 2K = p^2/M = 1$.

In this numerical test of the dynamical partition function versus a classical one, we consider seven different state points, all with the same values of N and T , but each with a different value of volume. To identify the correct classical ensemble, we need to consider the physical transformation that takes one of these systems into another. Clearly, changing the volume implies doing work on the system, and some of this work will be transformed into heat. To maintain the temperature at a fixed value, the volume change must take place while the system is in contact with a heat bath. Although the dynamical mechanism of the heat bath is not explicit in our numerical scheme, it is implicit in the different systems that we choose to compare. Therefore the appropriate ensemble for us is the canonical ensemble, and we use Eq. (3) to calculate the change in the canonical partition function as a function of volume (or spacing w). Integration Eq. (3) with respect to the volume at constant T and $N = 2$, we can calculate the change in the partition function for a given change in volume V ,

$$\ln Z(V_1) - \ln Z(V_0) = \int_{V_0}^{V_1} dV \frac{p}{kT} = (N - 1) \ln \left(\frac{V_1}{V_0} \right) + \int_{V_0}^{V_1} dV \frac{p^\phi}{kT} \quad (12)$$

Table I. Dynamical Partition Function

w	Length	Cycles	V	Z_{Shanks}
0.025	12	2602	3.5512	0.3157
0.05	12	7792	3.6395	0.2936
0.1	12	25918	3.8192	0.3504
0.150	11	25032	4.0000	0.4596
0.2	10	25842	4.1916	0.5560
0.236	10	51072	4.3301	0.6266
0.300	10	165150	4.5813	0.7387

From the accurate polynomial approximation for the potential contribution to the pressure obtained previously⁽²⁾ we can easily compute the change in the logarithm of the partition function as a function of the volume.

To test whether the dynamical partition function constructed in Eq. (8) generates the thermodynamic properties of the Lorentz gas, we numerically evaluate $Z_d(V)$ at seven different volumes. This involves an extrapolation to infinite n based on a range of finite values of n .⁽²⁾ Our results are presented in Table I, where the column labeled Z_{Shanks} represents the values of Z_d for the highest n , after they have been processed with a Shanks transformation. The column labeled Cycles gives the number of cycles obtained at the largest length. The accuracy of these estimates of the partition function varies. At small spacings there are significant contributions to the periodic orbit expansions at larger lengths, whereas at higher spacings convergence is achieved at smaller lengths, but here there are sampling problems due to the much larger number of cycles.

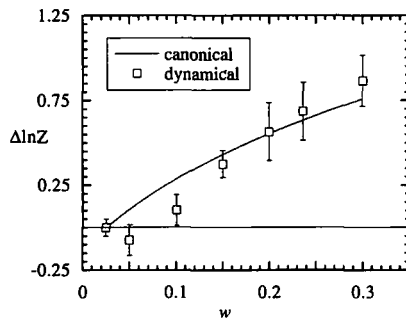


Fig. 2. Changes in the partition function. The continuous curve represents the change of the canonical partition function obtained by integrating the pressure, using Eq. (11). The squares represent the change in the dynamical (periodic orbit expansion) partition function, using Eq. (8).

To compare with the standard thermodynamic method of Eq. (11), we present the change in the logarithm of the partition function as a function of spacing in Fig. 2. We choose $w_0 = 0.025$ as our reference point, defining $\Delta \ln Z(w_0) = 0$. The results obtained by integrating the p^ϕ (referred to as canonical in Fig. 2) are highly accurate due to the accuracy of the polynomial approximation. The error bars have been computed using the Z_{Shanks} values of Table I and linear extrapolations in $1/n$.⁽²⁾

4. CONCLUSIONS

The proposed dynamical partition function gives results that oscillate about the canonical partition function (obtained by integrating the pressure). The canonical ensemble is needed when we move between state points at fixed temperature, which is achieved by contact with a heat bath. Figure 2 suggests, because of the consistency of the slopes of the canonical and dynamical partition function results, that the dynamical partition function is a likely candidate as a generating function for the thermodynamics of the Lorentz gas. The numerical difficulties in both calculating and enumerating all UPOs of length 12 are formidable and probably near the limit of our present generation of workstations. It would require a considerable increase in both storage and wordlength to extend these calculations.

The convergence of orbital measures to the natural measure for Axiom A flows⁽³⁾ is in the weak sense, i.e., the explicit form of the natural measure need not equal the pointwise limit of the orbital ones, although averages calculated here using the two measures are the same. Here we demonstrate that the UPO measure and the microcanonical ensemble give the same averages for the Lorentz gas. If this were true for an arbitrary phase variable, then we would be able to choose a phase variable which is equal to unity on phase element $d\Gamma$ and zero elsewhere. The UPO average of this variable would then equal the microcanonical probability of $d\Gamma$, and we would have a dynamical basis for the assumption of equal *a priori* probability.

Measures can be defined in terms of the averages that they produce on a given function space (the set of observables); thus, measures which are equivalent on a restricted function space may turn out to be different if the set of observables is enlarged. For instance in ergodic theory one proves that the microcanonical ensemble is the natural measure for the Lorentz gas if the observables are continuous functions of phase. However, our measure which is also dynamically defined, can be shown to be different from the microcanonical one if we enlarge the set of observables to contain characteristic functions of (Lebesgue) measurable sets. Nonetheless, we claim that although different points must be given different weights, the

weight given to an element of phase-space is equal to the that given to any other element (with the same volume). The reason is that every element of finite size in phase-space contains infinitely many points of different UPOs whose weights balance each other so as to produce a uniform distribution. Therefore, our UPO-derived measure turns out to be equivalent to the microcanonical ensemble for all choices of “reasonable” sets of observables (e.g., continuous functions of phase). As the UPOs are completely determined by the dynamics, we argue that every distribution other than the microcanonical measure would not have a dynamical basis, even if they produce the same thermodynamic averages.

ACKNOWLEDGMENTS

We thank Dr. N. Chernov for some insightful remarks. This work has been supported by the Australian Research Council (A69131116). L. R. gratefully acknowledges partial support from GNFM-CNR (Italy), while E.G.D.C. is indebted to the U.S. Department of Energy for support under contract DE-FG02-88-GR13847.

REFERENCES

1. R. C. Tolman, *The Principles of Statistical Mechanics* (Oxford University Press, Oxford, 1938); C. J. Thompson, *Mathematical Statistical Mechanics* (Macmillan, New York, 1972).
2. G. P. Morriss and L. Rondoni, *J. Stat. Phys.* **75**:553 (1994).
3. W. Parry, *Commun. Math. Phys.* **106**:267 (1986).
4. P. Cvitanovic, P. Gaspard, and T. Schreiber, *Chaos* **2**:85 (1992).
5. W. N. Vance, *Phys. Rev. Lett.* **69**:1356 (1992).
6. C. Grebogi, E. Ott, and J. A. Yorke, *Phys. Rev. A* **37**:1711 (1988).
7. D. Auerbach, P. Cvitanovic, J.-P. Eckman, G. Gunaratne, and I. Procaccia, *Phys. Rev. Lett.* **58**:2387 (1987).
8. J. H. Hannay and A. M. Ozorio de Almeida, *J. Phys. A* **17**:3429 (1984).
9. P. Gaspard and D. Alonso Ramirez, *Phys. Rev. A* **45**:8383 (1992).
10. Ya. G. Sinai, *Russ. Math. Surv.* **25**:137 (1970).
11. D. Ruelle, *Thermodynamic Formalism* (Addison-Wesley, Reading, Massachusetts, 1978).
12. D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic Press, London, 1990).