Lyapunov Exponents and KS Entropy for the Lorentz Gas at Low Densities

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The Lyapunov exponents and the Kolmogorov-Sinai entropy for a two dimensional Lorentz gas at low densities are defined for general non-equilibrium states and calculated with the use of a Lorentz-Boltzmann type equation. In equilibrium the density dependence of these quantities predicted by Krylov, is recovered and explicit expressions are obtained . The relationship between KS entropy, Lyapunov exponents and diffusion coefficients, developed by Gaspard and Nicolis is generalized to a wide class of non-equilibrium states.

A standard model for studying irreversible processes in classical fluids is the Lorentz gas, consisting of a system of fixed hard disk or hard sphere scatterers placed at random in space, with a particle that moves freely between elastic collisions with the scatterers [1]. This model of diffusion has been the object of considerable interest, as a non trivial system with irreversible behavior, accessible both to mathematical analysis, and to a study of its transport properties by means of kinetic theory. It has been possible to provide rigorous proofs that, under reasonable physical assumptions, the Lorentz gas is at least a K- system and that the periodic Lorentz gas is a Bernoulli system [2,3]. This implies that the Lorentz gas has a well defined equilibrium state and that a suitably defined initial distribution will approach equilibrium.

The purpose of this letter is to present a calculation of quantities that characterize the dynamic properties of random Lorentz gases. We illustrate the method for the two dimensional case and compute the positive Lyapunov exponent λ^+ and the Kolmogorov - Sinai entropy, h_{KS}, for such a model in the limit of low density of randomly placed scatterers for two cases: (1) The system is large and has periodic boundaries (which we eventually allow to move off to infinity); and (2) The scatterers are distributed over a large finite area with an absorbing boundary. The first case will allow us to verify a conjecture of Krylov, discussed by Sinai and others [4], that $\lambda^+ \sim \tilde{n} \ln \tilde{n}$, where $\tilde{n}$ is the reduced density of scatterers, $\tilde{n} = na^2$, with n the density of the scatterers, and a their radius. The second case will show that the Lyapunov exponents and Kolmogorov - Sinai entropy for open systems have finite size corrections that can be related to the coefficient of diffusion, as suggested by Gaspard and Nicolis [5,6].

The starting point for our analysis is a result due to Sinai [2], for the curvature of an expanding "wave front" that describes the unstable manifold of the phase space trajectory for the moving particle in the positive time direction. For our purposes the essential ingredients in Sinai's formula are: (a) The curvature, κ, is the inverse of the radius of curvature, ρ , i.e., $\kappa = (\rho)^{-1}$. In the present, two dimensional case ρ may be interpreted simply as the distance of two infinitesimally close particle trajectories to their mutual intersection point, which, for the unstable manifold, has to be located in the backward direction. (b) Between collisions ρ increases linearly with time as vt where v is the (constant) speed of the moving particle. (c) Whenever the particle collides with a scatterer, there is an instantaneous change in the curvature according to $\kappa^+ = \kappa^- + \frac{2}{acos\phi}$ where $\kappa^+ = 1/\rho^+$ is the curvature immediately after the collision, $\kappa^- = 1/\rho^-$ is the curvature immediately before the collision, and ϕ is the angle of incidence in the collision of the particle with a scatterer, with $-\pi/2 \le \phi \le \pi/2$ (see Fig. 1).

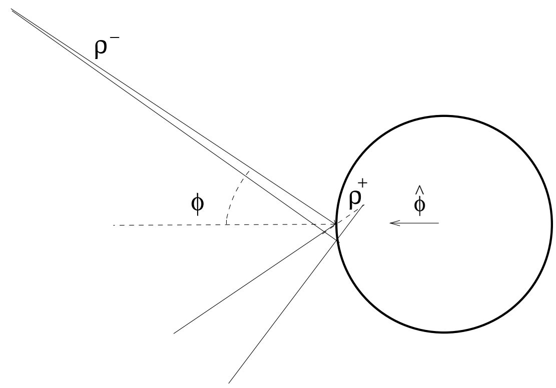

FIG. 1. The change in the radius of curvature at a collision

Suppose the trajectories go through collisions at times $\tau_1, \tau_2, \cdots, \tau_n, \cdots$. Then the radius of curvature at time t between τ_n and τ_{n+1} satisfies the relation

$$\rho(t) = v\tau + \left(\frac{2}{acos\phi_n} + \frac{1}{\rho_n^-}\right)^{-1} \tag{1}$$

where $\tau = t - \tau_n$, and ρ_n^- is the radius of curvature immediately before the collision with a scatterer at time τ_n.

The relation between the curvature $\rho(t)$ and the positive Lyapunov exponent characterizing a particular trajectory of the moving particle for the two dimensional case discussed here, is given by the time average

$$\lambda^+(\mathbf{r},\mathbf{v}) = \lim_{t\to\infty} \frac{v}{t}\int_0^t \frac{1}{\rho(\mathbf{r}(\tau),\mathbf{v}(\tau),\rho_0,\tau)} d\tau \tag{2}$$

In eq.(2), the initial radius of curvature ρ_0 may be taken to be any convenient value, since the initial value will be unimportant for the time average. In general this time average will be difficult to compute. However if the system is ergodic, the time average can be replaced by an ensemble average over all allowed positions and velocities of the moving particle, i.e.

$$\lambda^+ = v\langle\frac{1}{\rho(\mathbf{r},\mathbf{v})}\rangle \tag{3}$$

where $\rho(\mathbf{r},\mathbf{v})$ is the limit of $\rho(\mathbf{r},\mathbf{v},t)$ for fixed final coordinates and $t\to\infty$ (this limit is independent of ρ_0). A further important simplification is obtained by averaging also over all allowed positions of scatterers (which we will assume to be non-overlapping). In that case we obtain an expression for λ^+ of the same form as eq.(3), but now the brackets imply an average over the scatterer positions as well as over the position and velocity of the moving particle. It is this expression that we wish to evaluate for the cases described above. For the case of a large system with periodic boundaries, there is no conceptual difficulty with imagining ρ to be generated by an infinite number of collisions in the past. For the open system, we consider the limit for $t\to\infty$ of the set of trajectories that do not escape through the boundaries of the system before time t. Gaspard and Nicolis identify these as taking place on the fractal repeller of the system. On this set of trajectories we can imagine an infinite number of past collisions generating ρ.

We calculate λ^+ using eq.(3) by expressing the average value in terms of a distribution function $P(\mathbf{r},\mathbf{v},\rho,t)$ such that $Pd\mathbf{r}d\mathbf{v}d\rho$ is the probablility of finding a particle in the indicated ranges of variables at time t . The Lyapunov exponent can be expressed in terms of P as

$$\lambda^+ = \lim_{t\to\infty}\frac{v}{N(t)}\int\frac{1}{\rho}P(\mathbf{r},\mathbf{v},\rho,t)\,d\mathbf{r}\,d\mathbf{v}\,d\rho \tag{4}$$

where $N(t) = \int P\,d\mathbf{r}\,d\mathbf{v}\,d\rho$. For the closed system the function P does not depend on $\mathbf{r},\mathbf{v}$, or t, but for the open system it does, as we shall see presently.

The probability distribution P changes in time both through free streaming of the moving particle and through its collisions with the scatterers. In a low density Lorentz gas these collisions occur with an average frequency $\nu = 2anv$. A collision of the moving particle with a scatterer produces an instantaneous change in the radius of curvature according to the result quoted in point (c) above. As a result of these considerations one can easily show that the time evolution of the probability distribution P is described by a Lorentz-Boltzmann type of equation, of the form

$$\begin{aligned}\{\partial/\partial t + \mathbf{v}\cdot\nabla\}P(\mathbf{r},\mathbf{v},\rho,t) &= -v\partial/\partial\rho P(\mathbf{r},\mathbf{v},\rho,t) + \\ &+\nu\{-P(\mathbf{r},\mathbf{v},\rho,t) + 1/2\int_{-\pi/2}^{\pi/2}d\phi\int_0^\infty d\rho'\cos\phi \\ &\delta(\rho - \frac{a\cos\phi/2}{1+a\cos\phi/2\rho'})P(\mathbf{r},\mathbf{v}',\rho',\mathbf{t})\}\end{aligned} \tag{5}$$

The first term on the right hand side of eq.(5) describes the change in ρ due to free streaming and the last two terms describe the changes in P resulting from collisions of the moving particle with scatterers. The loss term assumes the simple form $-\nu P$ because both the speed of the moving particle and the density of the scatterers are constants. The gain term counts collisions transforming precollisional coordinates $(\mathbf{r}',\mathbf{v}',\rho')$ into postcollisional coordinates $(\mathbf{r},\mathbf{v},\rho)$. The relationship between $\mathbf{v}$ and $\mathbf{v}'$ is given by $\mathbf{v}' = \mathbf{v} - 2(\mathbf{v}\cdot\hat{\phi})\hat{\phi}$, where $\hat{\phi}$ is the unit vector in the direction from the center of the scatterer to the point of impact of the moving particle at the collision (see Fig.1). The usual Lorentz-Boltzmann equation [1] is obtained from eq.(5) by integrating it over all values of ρ, provided P satisfies the condition that $P\to 0$ as $\rho\to 0$. We require that the solutions to eq.(5) satisfy this condition, since the free streaming current always leads to larger ρ, and there is no influx at the origin from negative values of ρ.

In this paper we only want to solve eq.(5) to lowest order in a systematic expansion in powers of the reduced density of scatterers, $\tilde{n} = na^2$. Since the typical values of ρ' in eq.(5) are of the order of the mean free path $\ell = v/\nu = 1/(2na)$, the term $a\cos\phi/\rho'$ occurring in the denominator in the delta function in eq.(5) is of order $\tilde{n}$ and may be neglected compared to 1. The corrections can be shown to be of relative order $\tilde{n}\ln\tilde{n}$. Then the integration over ϕ can easily be performed and eq.(5) reduces to the simpler form

$$\begin{aligned}&\{\partial/\partial t + \mathbf{v}\cdot\nabla\}P(\mathbf{r},\mathbf{v},\rho,t) = \\ &= -v\partial/\partial\rho\, P + \nu\{-P + \frac{1}{a}\Theta(1-\sigma)\frac{\sigma}{(1-\sigma^2)^{1/2}} \\ &\int_0^\infty d\rho'[P(\rho',\mathbf{r},\mathbf{v}'_+,t) + P(\rho',\mathbf{r},\mathbf{v}'_-,t)]\}\end{aligned} \tag{6}$$

where Θ is the unit step function and $\sigma = 2\rho/a$. The velocities $\mathbf{v}'_\pm$ both are precollisional velocities, with scattering vectors $\hat{\phi}_\pm$ satisfying $\mathbf{v}\cdot\hat{\phi}_\pm = v\sigma$.

We first consider the equilibrium system with periodic boundary conditions. In this case the solution to eq.(6) does not depend on $\mathbf{r},\mathbf{v}$ or t, and this equation reduces to

$$(v\partial/\partial\rho + \nu)P(\rho) = \frac{2\,\nu\,\sigma\Theta(1-\sigma)}{a(1-\sigma^2)^{1/2}}\int_0^\infty d\rho' P(\rho') \tag{7}$$

The solution to this equation is simply obtained as $P(\rho) = c_0 n_m^e f_0(\rho)\delta(|\mathbf{v}| - v)$ where n_m^e is the equilibrium density of the moving particle, and $c_0 = 1/(2\pi v)$ is the normalization of the velocity distribution. To lowest order in $\tilde{n}$, f_0 is

$$\begin{aligned} f_0(\rho) &= (1/\ell)e^{-\rho/\ell} && \rho > a/2 \\ f_0(\rho) &= (1/\ell)[1 - (1-\sigma^2)^{1/2}] && \rho < a/2 \end{aligned} \tag{8}$$

Notice that up to corrections of relative order $\tilde{n}$, this solution is continuous at $\rho = a/2$, and satisfies the proper normalization condition, $\int_0^\infty P(\rho)d\rho = c_0 n_m^e \delta(|\mathbf{v}| - v)$.

From eqs.(4) and (8) the Lyapunov exponent follows immediately as

$$\lambda^+ = 2nav(1 - \ln 2 - C - \ln \tilde{n}) \qquad \text{for } \tilde{n} \ll 1 \tag{9}$$

where C is Euler's constant. By Pesin's theorem for closed systems, it follows that $h_{KS} = \lambda^+$. This result agrees with the conjecture of Krylov, and we have determined both the terms of order $\tilde{n}$ ln $\tilde{n}$ as well as of order $\tilde{n}$. The coefficient of the $\tilde{n}$ ln $\tilde{n}$ term agrees with an similar result, [7], [8], obtained for the periodic case as the radius of the disks becomes small. The coefficient of the order $\tilde{n}$ term is new.

Next we turn to the calculation of the Lyapunov exponent for the fractal set of trapped trajectories on a finite area with absorbing boundary [9]. Since almost every trajectory of the moving particle starting on this area leads to escape, we have to construct a non-equilibrium solution of eq.(6) and compute λ^+ using eq.(4), taking the limit $t \to \infty$. The appropriate solution of eq.(6) is the Chapman-Enskog hydrodynamic solution [10] which is completely determined by the local density of the moving particle, and the density gradients. Thus, we look for solutions of the form

$$\begin{aligned} P(\mathbf{r},\mathbf{v},\rho,t) = c_0\delta(|\mathbf{v}| - v)\{p_0(\mathbf{r},\mathbf{v},\rho,t) + \\ + p_1(\mathbf{r},\mathbf{v},\rho,t) + p_2(\mathbf{r},\mathbf{v},\rho,t) + \cdots\} \end{aligned} \tag{10}$$

where p_i is proportional to the $i-th$ gradient of the local density of the moving particle. The lowest order solution is the local equilibrium solution

$$p_0(\mathbf{r},\mathbf{v},\rho,t) = n_m(\mathbf{r},t)f_0(\rho) \tag{11}$$

where f_0 is given by eq.(8). The first order equation is obtained by consistently keeping all terms in eq.(6) which are first order in the gradients, and is given by

$$\begin{aligned} & f_0(\rho)\,(\partial^{(1)}/\partial t + \mathbf{v}\cdot\nabla)\,n_m(\mathbf{r},t) = \\ & = -v\partial/\partial\rho\, p_1(\mathbf{r},\mathbf{v},\rho,t) + \nu[-p_1(\mathbf{r},\mathbf{v},\rho,t) + \frac{1}{a}\Theta(1-\sigma) \\ & \frac{\sigma}{(1-\sigma^2)^{1/2}}\int_0^\infty d\rho'[p_1(\mathbf{r},\mathbf{v}'_+,\rho',t) + p_1(\mathbf{r},\mathbf{v}'_-,\rho',t)] \end{aligned} \tag{12}$$

Here the term $\partial^{(1)}/\partial t\, n_m(\mathbf{r},\mathbf{t})$ is the first order gradient term in the hydrodynamic equation for the local density of the moving particle. This term is zero, and is dropped. As the collision operator does not change the tensorial character in $\mathbf{v}$ of the functions on which it operates, we may set $p_1(\mathbf{r},\mathbf{v},\rho,t) = f_1(\rho)\,\mathbf{v}\cdot\nabla n_m(\mathbf{r},t)$, with f_1 satisfying

$$f_0 + (v\partial/\partial\rho + \nu)f_1 = \Theta(1-\sigma)\frac{2\nu\sigma(1-2\sigma^2)}{a(1-\sigma^2)^{1/2}}\int_0^\infty d\rho' f_1(\rho') \tag{13}$$

The solution to eq.(13) can be determined to lowest order in $\tilde{n}$ by noticing that f_1 must be continuous at $\rho = a/2$ since the right hand side of the equation contains no delta functions. We then find that

$$f_1(\rho) = -(1/v\ell)\rho e^{-\rho/\ell} + (1/4v)e^{-\rho/\ell} \qquad \rho > a/2 \tag{14}$$

$$f_1(\rho) = (1/4v)\{1 - (1-\sigma^2)^{1/2}(1+2\sigma^2)\} \qquad \rho < a/2 \tag{15}$$

Again, we have used the condition that $f_1(\rho) \to 0$ as $\rho \to 0$. Proceeding to second order, we find that application of $\mathbf{v}\cdot\nabla$ to p_1 leads to a term that as a function of $\mathbf{v}$ can be separated into a traceless tensor of the second degree in $\mathbf{v}$ and a scalar part. Consequently p_2 can be separated into a scalar part p_2^s and a part proportional to the traceless tensor $\mathbf{vv} - (v^2/2)\mathbf{1}$. For the determination of the Lyapunov exponent only the scalar term is important since the traceless tensor part yields zero on integration over $\mathbf{v}$. Thus we write

$$p_2^s(\mathbf{r},\mathbf{v},\rho,t) = \nabla^2 n_m(\mathbf{r},t)f_2(\rho) \tag{16}$$

and we find that $f_2(\rho)$ satisfies the equation

$$f_0(\rho)D + (v^2/2)f_1(\rho) + (\nu + v\partial/\partial\rho)f_2(\rho) = 0 \tag{17}$$

Here we have imposed a solubility condition in the Chapman-Enskog method which requires that $\int_0^\infty f_2\,d\rho = 0$. The quantity D, appearing in this equation is the low density value of the coefficient of diffusion of the moving particle, which is given by $D = (3/8)\ell v$.

From eqs.(4,11 and 16) one finds the positive Lyapunov exponent as

$$\lambda^+ = \lambda_0^+ + \lim_{t\to\infty}\frac{\kappa_2\, v\int\nabla^2 n_m(\mathbf{r},t)d\,\mathbf{r}}{N(t)} \tag{18}$$

where λ_0 is the closed system value, (9), and $\kappa_2 = \int_0^\infty 1/\rho\, f_2(\rho)\,d\,\rho = -\ell/4$.
Using Fick's law expressing the diffusion current as $\mathbf{j}(\mathbf{r},t) = -D\nabla n_m(\mathbf{r},t)$, defining the escape rate as $E = \lim_{t\to\infty} 1/N(t)\int_\Lambda \mathbf{j}(\mathbf{r},\mathbf{t})\cdot\hat{\mathbf{n}}\,\mathbf{dS}$, with Λ denoting the boundary of the system and $\hat{\mathbf{n}}$ the unit vector pointing outward from the boundary, and employing Gauss's law, one can reexpress λ^+ in terms of E as

$$\lambda^+ = \lambda_0^+ - \kappa_2\, vE/D = \lambda_0^+ + (2/3)\,E. \tag{19}$$

We have thus shown that the Lyapunov exponent for a random, two dimensional Lorentz gas can be calculated for both closed and open systems, that this calculation can be done using standard methods from the kinetic theory of gases, and that the results are consistent with the escape-rate formalism employed by Gaspard and Nicolis in their discussion of diffusion [5]. Finally we can obtain the KS entropy for the system with absorbing boundaries from the well-known relation [11] $h_{KS} = \sum_{\alpha}' \lambda_\alpha - E$, where the sum runs over the positive Lyapunov exponents only. Collecting the previous results we find

$$h_{KS} = h_{KS}^{(0)} - (1/3)\, E \tag{20}$$

with $h_{KS}^{(0)}$ the KS entropy of the closed system.

We conclude with a few brief remarks. (1) This method can be extended to higher dimensions, to higher densities, and to more complicated processes where all of the particles are moving. One needs to work out the kinetic theory for the appropriate Boltzmann-like equation to do so. Work in these directions is in progress. (2) One of the most remarkable conclusions to be drawn is that for a two dimensional Lorentz gas the Lyapunov exponents and KS entropy can be expressed as ensemble averages of a static local quantity, the local curvature $1/\rho(\mathbf{r}, \mathbf{v})$. In how far this can be generalized to higher dimensional systems is presently under investigation. For the two dimensional Lorentz gas Lyapunov exponents and KS entropy can be defined for arbitrary non-equilibrium ensembles through eq.(3), and the approach to equilibrium of these quantities can be obtained from the time evolution of these ensembles. (3) In our derivation of the relationship (19) between the nonequilibrium positive Lyapunov exponent and the escape rate we only used Fick's law and we did not have to specify the precise nature of the boundary conditions. Hence, this relationship is generally valid, as long as the state of the system can be described by a Chapman-Enskog type hydrodynamic distribution function. The system size must be large so that higher order gradient and boundary layer corrections may be neglected. We may also conclude that deviations from the equilibrium values occur only for a non-vanishing escape rate, at least in the absence of external force fields. (4) Our results are the analogs for a continuous system of closely related calculations for Lorentz lattice gases by Ernst, Dorfman, Nix and Jacobs, reported in a companion paper [12]. The Lorentz lattice gas is simpler to study since it can be studied as a Markov chain, and it is very amenable to computer simulations. The two systems are close in spirit, and the methods to treat them have many similar features. Finally, it is a pleasure to note that Boltzmann's equation is useful for determining features of the chaotic dynamics of many particle systems that are ultimately responsible for the irreversible behavior that Boltzmann understood at a very deep level.

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[1] E. H. Hauge, in Lecture Notes in Physics **31**, 337 (1974), G. Kirczenow and J. Marro, eds., Springer Verlag, Berlin; E. G. D. Cohen in *Colloques Internationaux C.R.N.S.*, No. 236, p.269 (1974).

[2] Ya. G. Sinai, Russ. Math. Surv. **25**, 137 (1970); Funct. Anal. Appl.**13**, 192 (1980); L. A. Bunimovich and Ya. G. Sinai, Comm. Math. Phys. **78**, 479 (1981); Ya. G. Sinai and N. I. Chernov, Russ. Math. Surv.**42**, 181, (1987); see also P. Gaspard, in *Quantum Chaos*, G. Casati, I. Guarneri, and U. Smilansky, eds. North-Holland, Amsterdam (1993), p.307.

[3] L. A. Bunimovich in *Dynamical Systems,II*, Ya. G. Sinai, ed. Springer Verlag, Berlin (1989), p. 151. G. Gallavotti and D. S. Ornstein, Comm. Math. Phys. **38**, 83, (1974). N. I. Chernov and C. Haskell, Erg. Th. and Dyn. Syst. (to appear).

[4] N. S. Krylov *Works on the Foundations of Statistical Physics*, Princeton U. Press, Princeton (1979); Ya. G. Sinai, *ibid.* p. 239. P. Gaspard and X.-J. Wang, Phys. Rept. **235**, 291, (1993).

[5] P. Gaspard and G. Nicolis, Phys. Rev. Lett. **65**, 1693, (1990).

[6] P. Gaspard and F. Baras, in *Microscopic Simulations of Complex Hydrodynamic Phenomena*,M. Maréschal and B. Holian.eds. Plenum Press, New York (1992), p.301; P. Gaspard and F. Baras (unpublished).

[7] B. Friedman, Y. Oono, and I. Kubo, Phys. Rev. Lett. **52**, 709, (1984).

[8] N. I. Chernov, Funct. Anal. Appl. **25**, 204, (1991).

[9] Here we assume that when properly normalized by the survival probability, the measure on the trapped trajectories approaches a well defined limit, determined by the Chapman-Enskog solution of the Lorentz-Boltzmann equation with the appropriate absorbing boundary conditions. This ought to be valid in the Boltzmann-Grad limit, though no proof is available, yet.

[10] S. Chapman and T. G. Cowling *Mathematical Theory of Non-Uniform Gases, 3rd. edition*, Cambridge U. Press, Cambridge (1970).

[11] J.-P. Eckmann and D. Ruelle, Rev. Mod. Phys. **57**, 617, (1985).

[12] M. H. Ernst, J. R. Dorfman, R. Nix, and D. Jacobs (unpublished)