LETTER

Non-equilibrium Lorentz gas on a curved space

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Abstract. The periodic Lorentz gas with external field and iso-kinetic thermostat is equivalent, by conformal transformation, to a billiard with expanding phase space and slightly distorted scatterers, for which the trajectories are straight lines. A further time rescaling allows one to keep the speed constant in that new geometry. In the hyperbolic regime, the stationary state of this billiard is characterized by a phase-space contraction rate, equal to that of the iso-kinetic Lorentz gas. In contrast to the iso-kinetic Lorentz gas case where phase-space contraction occurs in the bulk, the phase-space contraction rate here takes place at the periodic boundaries.

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Over the last twenty years, the study of time-reversible dissipative systems with chaotic dynamics as mechanical models of non-equilibrium stationary processes has played an important role in shaping our understanding of the connections between irreversible macroscopic processes and the reversible dynamics that underlie them at the microscopic level; see [1] and references therein. Among other large deviation relations, the fluctuation theorem [2,3] is a central result of this approach. Related results have appeared since then [4,5], which have been put to the test experimentally in small circuits and biological molecules; see [6] and references therein.

The forced periodic Lorentz gas with Gaussian iso-kinetic thermostating was first proposed by Moran and Hoover [7] as such a time-reversible dissipative chaotic model for conduction, where irreversibility manifests itself in the fractality of phase-space distributions.

A rigorous analysis of that system was later provided by Chernov *et al* [8], establishing a relation between the sum of the Lyapunov exponents and the entropy production rate of this system. The thermostat is here a mechanical constraint, chosen according to Gauss's principle of least constraint, which acts so as to remove the energy input from an external field [9]. Under this constraint, the kinetic energy remains constant and thus fixes the temperature of the system; no interaction with a hypothetical environment is needed in order to achieve thermalization. Rather the Gaussian thermostat causes dissipation in the bulk. Due to the presence of a regular array of circular scatterers on which non-interacting particles collide elastically, this system sustains a chaotic regime, at least so long as the external forcing is not too strong. As shown in [8], this model has a unique natural invariant measure, with one positive and one negative Lyapunov exponents, whose sum is negative—a signature of the fractality of the invariant measure—and identified as minus the entropy production rate [10]. The comparison with the corresponding phenomenological expression provides a relation between the phase-space contraction rate and conductivity.

As will be reviewed shortly, the trajectories of the iso-kinetic billiard are integrable from one collision to the next. It was shown by Wojtkowski [11] that there exists a conformal transformation on the complex plane that transforms those curved trajectories into straight lines. Formally, this amounts to introducing a metric, specified according to the conformal transformation, which yields an identification between the Gaussian iso-kinetic trajectories and the geodesics of a torsion free connection, called the Weyl connection, for which the metric is preserved under parallel transport. This is a natural generalization of the symplectic formalism for the Gaussian iso-kinetic motion introduced by Dettmann and Morriss [12]. The corresponding billiard, whose trajectories follow the geodesics of the Weyl connection, and undergo elastic collisions when they reach the boundary, is referred to as the billiard W-flow. For our purpose, it will be sufficient to focus our attention on the conformal transformation itself, leaving aside the formal aspects of this geometric construction, which we will henceforth loosely refer to as Weyl geometry.

In what follows, we will present the details of this conformal transformation and study the dynamics of the billiard. Our main observation is that the bulk dissipation of the iso-kinetic Lorentz billiard, which accounts for the positive entropy production rate, disappears under the conformal map, after time reparametrization. The phase-space contraction rate and its identification with the entropy production rate are nevertheless recovered because of the periodic boundary conditions, which, under the conformal map,
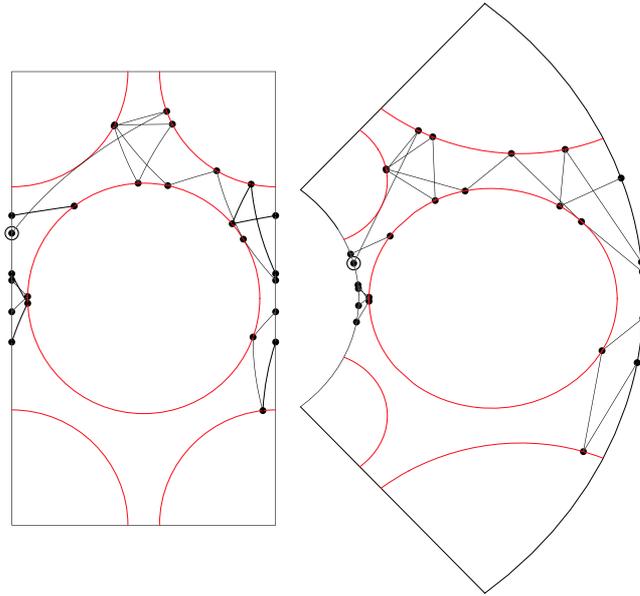
Figure 1. Left: unit cell with a typical trajectory, corresponding to the external field $\epsilon = 1$; right: the image of that cell and trajectory under the conformal map (7). The initial condition is marked by a circled dot.

induce a phase-space contraction rate which, on average, is equal to the bulk dissipation of the iso-kinetic Lorentz billiard. We mention that a billiard with a similar mechanism of contraction of phase-space volumes at the borders was considered in [13]. However the connection to iso-kinetic dynamics was not discussed there.

We consider the two-dimensional iso-kinetic periodic Lorentz channel with constant external field of magnitude ϵ. Due to the periodicity of this system, the dynamics can be studied in a unit cell with periodic boundary conditions, as displayed on the left panel of figure 1. This cell is an open rectangular domain, centred at the origin, with one disc at the cell's centre, and four others at its summits $(\pm 1/2, \pm\sqrt{3}/2)$. All the discs have identical radii, which we denote by σ, chosen so as to satisfy the finite horizon condition, i.e. $\sqrt{3}/4 < \sigma < 1/2$. The width of the cell is here taken to be unity, and its height $\sqrt{3}$. Periodic boundary conditions apply at $x = \pm 1/2$ and reflection at $y = \pm\sqrt{3}/2$. The direction of the external field is taken towards the positive x direction. Thus particles typically tend to move in that direction, winding around the cell from one boundary to the other.

Let (x_t, y_t) denote the coordinates of the particle at time t, and let θ_t denote the velocity angle, measured with respect to the x-axis. Assume $p^2 \equiv \dot{x}_t^2 + \dot{y}_t^2 \equiv 1$, which we take as the definition of the temperature. In between collisions the equations of motion are specified by

$$\dot{x}_t = \cos\theta_t, \tag{1}$$

$$\dot{y}_t = \sin\theta_t, \tag{2}$$

$$\dot{\theta}_t = -\epsilon\sin\theta_t, \tag{3}$$

with the solutions

$$x_t = x_0 + \frac{1}{\epsilon} \log \frac{\sin \theta_0}{\sin \theta_t}, \tag{4}$$

$$y_t = y_0 + \frac{\theta_0 - \theta_t}{\epsilon}, \tag{5}$$

$$\theta_t = 2 \arctan \left[\tan \frac{\theta_0}{2} \exp(-\epsilon t) \right]. \tag{6}$$

When the trajectory collides with a disc, θ_t changes according to the rules of elastic collisions.

Let $z = x + \mathrm{i}y$ and $f(z) = -\epsilon(x + \mathrm{i}y)$. That is, f is a holomorphic function whose real part is specified by the potential associated with the external field. According to Wojtkowski [11], the conformal mapping

$$F(z) = \int \exp[-f(z)] \, \mathrm{d}z \tag{7}$$

takes the trajectories (4), (5) into straight lines. This is to say $F(t) \equiv F(z_t)$ is a straight line in the complex plane. Furthermore, since the transformation is conformal, the elastic collisions are mapped into elastic collisions. The periodic boundary conditions are modified under this map, as will be discussed shortly.

The map (7) takes a point with coordinates (x, y) to the point (u, v) in the complex plane,

$$\begin{aligned} x + \mathrm{i}y \mapsto u + \mathrm{i}v &= F(x + \mathrm{i}y), \\ &= \frac{1}{\epsilon} \{ \exp[\epsilon(x + \mathrm{i}y)] - 1 \}. \end{aligned} \tag{8}$$

Note that the term $-1/\epsilon$ was introduced so as to keep the origin fixed under the transformation.

We show that trajectories are straight lines in the (u, v) plane and identify their slopes. To that end, we compute the time derivative of $F(z_t)$ with $z_t = x_t + \mathrm{i}y_t$. From equations (1)–(3),

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} F(z_t) &= \exp[\epsilon(x_t + \mathrm{i}y_t)] \frac{\mathrm{d}}{\mathrm{d}t}(x_t + \mathrm{i}y_t), \\ &= \exp[\epsilon(x_t + \mathrm{i}y_t)] \exp(\mathrm{i}\theta_t), \\ &= \exp(\epsilon x_t) \exp[\mathrm{i}(\theta_t + \epsilon y_t)]. \end{aligned} \tag{9}$$

Notice that $\phi_t \equiv \theta_t + \epsilon y_t$ is a conserved quantity, as is immediately seen from equation (5). If we further change the time variable t to s, such that

$$\mathrm{d}s = \exp(\epsilon x_t) \, \mathrm{d}t, \tag{10}$$

we can write

$$\frac{\mathrm{d}}{\mathrm{d}s}(u_s + \mathrm{i}v_s) = \exp(\mathrm{i}\phi_0), \tag{11}$$

which is to say (u_s, v_s) is a straight line trajectory of slope $\tan(\phi_0)$, as announced, and constant speed. This result may indeed have been anticipated, since the transformation

to the new set of variables coincides with the one for which the iso-kinetic trajectories are transformed into geodesics of the metric $\exp(2\epsilon x)(\mathrm{d}x^2 + \mathrm{d}y^2)$, see [12].

Thus, in terms of the (u, v, ϕ) variables, the time evolution of trajectories between collisions is specified according to

$$u_s + \mathrm{i}v_s = u_0 + \mathrm{i}v_0 + \mathrm{e}^{\mathrm{i}\phi_0}s, \tag{12}$$

$$\phi_s = \phi_0. \tag{13}$$

The time reparametrization (10) introduces a new timescale, which is natural in the new geometry. However it depends on the details of the trajectory. For future reference, we will make a distinction between this *natural* time s and the *physical* time t. We integrate equation (10) in order to express the natural time variable, s, in terms of the physical one, t:

$$s = [(u_0 + 1/\epsilon)\cos\phi_0 + v_0\sin\phi_0][\cosh(\epsilon t) - 1] + \sqrt{(u_0 + 1/\epsilon)^2 + v_0^2}\,\sinh(\epsilon t). \tag{14}$$

As opposed to the Gaussian iso-kinetic trajectories, the phase-space volumes are obviously preserved along the trajectories of equations (12) and (13). The time variables are however different and, as is clear from equation (14), phase-space volumes are not preserved when the trajectories are parametrized according to the physical time t.

To make the comparison clearer, we first consider the Gaussian iso-kinetic dynamics, which maps trajectories $(x_0, y_0, \theta_0) \mapsto (x_t, y_t, \theta_t)$ according to equations (4)–(6). This map contracts phase-space volumes, with a rate given by minus the logarithm of the Jacobian of the application:

$$\begin{aligned}
\left|\partial_{(x_0, y_0, \theta_0)}(x_t, y_t, \theta_t)\right| &= \partial_{\theta_0}\theta_t, \\
&= (\cosh\epsilon t + \cos\theta_0\sinh\epsilon t)^{-1}, \\
&= \exp[\epsilon(x_0 - x_t)],
\end{aligned} \tag{15}$$

i.e. $\epsilon(x_t - x_0)$ is the phase-space contraction rate of the trajectory taking (x_0, y_0, θ_0) to (x_t, y_t, θ_t).

In the Weyl geometry of the billiard, on the other hand, the phase-space contraction rate of the physical time trajectory $(u_0, v_0, \phi_0) \mapsto (u_t, v_t, \phi_t)$ is minus the logarithm of the Jacobian,

$$\begin{aligned}
\left|\partial_{(u_0, v_0, \phi_0)}(u_t, v_t, \phi_t)\right| &= |\partial_{u_0, v_0}(u_t, v_t)|, \\
&= \cosh\epsilon t + \frac{(u_0 + 1/\epsilon)\cos\phi_0 + v_0\sin\phi_0}{\sqrt{(u_0 + 1/\epsilon)^2 + v_0^2}}\sinh\epsilon t, \\
&= \frac{\sqrt{(u_t + 1/\epsilon)^2 + v_t^2}}{\sqrt{(u_0 + 1/\epsilon)^2 + v_0^2}}.
\end{aligned} \tag{16}$$

This is the inverse of equation (15), as is easily checked. Therefore, so long as the timescales are the same, the phase-space volume contraction changes sign, going from the dynamics of the iso-kinetic billiard to that of the W-flow. Moreover minus the logarithm of the latter expression yields $\epsilon(u_0 - u_t)$ only to first order in ϵ. The reason for this is connected to the transformation law of x, equation (8): $x = 1/\epsilon \log\sqrt{(u + 1/\epsilon)^2 + v^2}$.

As remarked by Dettmann and Morriss [12], the periodic boundary conditions break the Hamiltonian structure of the billiard in the Weyl geometry. Indeed, they do not preserve phase-space volumes as we now show.

In order to analyse the billiard trajectories in the Weyl geometry, we must first consider the transformation of the unit cell under the conformal map, equation (8), as shown in the right panel of figure 1. It is straightforward to check the rectangular cell is mapped to a trapezoidal figure with curved lateral sides, and the discs to slightly distorted, flattened ones. Here are the parametric equations of these elements:

upper/lower sides: $\quad \left\{ u + \mathrm{i}v = \epsilon^{-1}[\exp(\epsilon t \pm \mathrm{i}\sqrt{3}\epsilon/2) - 1], \; -1/2 \leq t \leq 1/2 \right\},$

right/left sides: $\quad \left\{ u + \mathrm{i}v = \epsilon^{-1}[\exp(\pm\epsilon/2 + \mathrm{i}\sqrt{3}\epsilon t) - 1], \; -1/2 \leq t \leq 1/2 \right\},$

central disc: $\quad \left\{ u + \mathrm{i}v = \epsilon^{-1}\{\exp[\epsilon\sigma\exp(\mathrm{i}\phi)] - 1\}, \; 0 \leq \phi \leq 2\pi \right\},$

outer discs: $\quad \left\{ u + \mathrm{i}v = \epsilon^{-1}\{\exp[\epsilon(\pm 1/2 \pm \mathrm{i}\sqrt{3}/2 + \sigma\exp(\mathrm{i}\phi))] - 1\}, \; 0 \leq \phi \leq 2\pi \right\}.$

Notice that the upper and lower borders are oblique lines of slopes $\pm\sqrt{3}\epsilon/2$, while the left and right borders are concentric arc-circles of centre $(-1/\epsilon, 0)$ and respective radii $\exp(\pm\epsilon/2)/\epsilon$. Thus, the periodic boundary conditions induce phase-space expansion/contraction as the variables u and v are rescaled by a factor $\exp(\pm\epsilon)$ when the trajectory crosses from left to right or right to left.

In order to analyse the ergodic properties of the W-flow, we turn to the definition of the Birkhoff coordinates of the Weyl billiard in the periodic cell, which specify the evolution of trajectories from one collision to the next (including collisions with the boundaries). Three coordinates are necessary here: ς, which denotes the arc length along the boundaries of the unit cell (walls and discs), ω, the modulus of the velocity vector, and ϖ, by which we denote the sinus of the angle between the outgoing trajectory and the normal to the obstacles' boundaries, that is the tangent component of the unit vector in the direction of the velocity. As a result, in the stationary state, so long as the regime is hyperbolic, there are three Lyapunov exponents which characterize the chaoticity of the Birkhoff map. We denote them by $\lambda_1 > \lambda_2 > \lambda_3$, where λ_1 and λ_3 are associated with the (ς, ϖ)-dynamics, and λ_2 to the ω-dynamics, corresponding to the direction of the flow, and which is zero as it will turn out.

We first consider the dynamics of ω. Here we have to make a distinction between the two time parametrizations. If, on the one hand, we integrate trajectories with respect to the physical time t, the modulus of the velocity is typically expanded in the bulk according to equation (16), while it is contracted at the opposite rate by the periodic boundary conditions. That the particle's velocity must be rescaled by a factor $\mathrm{e}^{\pm\epsilon}$ at the periodic boundaries can be seen from the expression of the velocity, given by equation (10), here expressed in terms of the variables u, v, ϕ,

$$\omega_t = \frac{\mathrm{d}}{\mathrm{d}t}s = \epsilon \left\{ [(u_0 + 1/\epsilon)\cos\phi_0 + v_0\sin\phi_0]\sinh(\epsilon t) + \sqrt{(u_0 + 1/\epsilon)^2 + v_0^2}\cosh(\epsilon t) \right\}. \quad (17)$$

This rescaling yields a contribution to λ_2 equal to[3] $-\epsilon J_c$, where J_c is the (signed) average number of boundary crossings per collision, i.e. the average drift velocity per collision, a

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[3] For definiteness we assume the particle density to be normalized to unity.

positive quantity. The other contribution occurs from the bulk, because of the dissipation that takes place along the trajectories, and is given by the logarithm of equation (16). As we noted by comparing it to equation (15), this contribution is opposite to the phase-space contraction rate of the iso-kinetic billiard along the image trajectory. The latter quantity is equal to the entropy production rate of the iso-kinetic Lorentz gas, given by the product of the applied force by the resulting drift current [8], i.e. ϵJ_c. Thus the bulk contribution to λ_2 is identical but opposite to the contribution due to the boundary conditions. Therefore,

$$\lambda_2 = 0. \tag{18}$$

If, on the other hand, we integrate the trajectories with respect to the natural time, i.e. with respect to s, the dynamics of ω are trivial. Indeed the velocity is constant in the bulk and remains so under the periodic boundary conditions. This is because the s increments are rescaled at the boundaries identically to the length increments, as can be seen from equation (17). Thus, trivially, we again retrieve $\lambda_2 = 0$.

As noticed earlier, equations (12) and (13), the dynamics of ς and ϖ preserves the phase-space volumes in the bulk. This remains so whether the time variable is s or t. Since the trajectories follow straight lines, the evolution of these two variables from one collision event to the next is the same, whether the velocity changes in the bulk or remains constant. However, as noted earlier, phase-space volumes are not preserved when the periodic boundary conditions apply. The arc-length coordinate is contracted by a factor $e^{\pm\epsilon}$. We can therefore write minus the sum of the two Lyapunov exponents associated with the dynamics of ς and ϖ as

$$-\lambda_1 - \lambda_3 = \epsilon J_c. \tag{19}$$

The total phase-space contraction rate is the sum of equations (18) and (19), equal to the product of the current multiplied by the amplitude of the external field. This is obviously the same result as was obtained for the iso-kinetic Lorentz billiard [8], which we did expect since the winding number, and hence the current J_c, are invariant under the conformal map. Table 1 summarizes our findings. Notice that the current J_c is here measured with respect to the collision dynamics. The identification between the phase-space contraction rate and the entropy production per unit time (in the regime of linear transport) can be done by substituting the average current per collision, J_c, by the corresponding average current per unit time, which we denote by J_t. This is straightforward since the two quantities differ only by a conversion factor, the average free flight time, or average time between collisions. On the other hand, it should be mentioned that the conversion to a current measured in units of s is not meaningful since this integration variable changes from one trajectory to another. Each trajectory travels with its own clock, which impedes a statistical interpretation.

To conclude, we have shown how the transformation of the Gaussian iso-kinetic Lorentz channel to a Weyl geometry maps the trajectories into straight lines with constant speed, so long as we rescale the time variable according to equation (10). The geometry of the cell is modified under this transformation. The vertical walls of the Lorentz channel are here replaced by concentric circles whose radii differ by a factor given by the exponential of the external field. The discs are also deformed and can even have concavities when the field strength becomes too large ($\epsilon > 1/\sigma$, which corresponds to the transition to a non-hyperbolic regime, as shown in [11]).

Table 1. Comparison of the different contributions to the phase-space contraction rate for the Gaussian iso-kinetic Lorentz gas and its two equivalent representations in the Weyl geometry, whether the integration variable is t, the physical time, or s, the natural time; equation (14). In the former case, the contraction of the velocity at the periodic boundaries compensates for the expansion of phase-space volumes in the bulk.

Dissipation	Bulk	Boundaries	Total
GIK LG	ϵJ_c	0	ϵJ_c
W-flow (t)	$-\epsilon J_c$	$2\epsilon J_c$	ϵJ_c
W-flow (s)	0	ϵJ_c	ϵJ_c

The average phase-space contraction rate, equal (at least in the small ϵ regime) to the entropy production rate, is here due to the application of the periodic boundary conditions. A remarkable consequence of this is that the calculation of the phase-space contraction, as well as its identification with the entropy production rate, is immediate.

It should be pointed out that the expression of the phase-space contraction rate, equation (19), makes no reference to the actual timescale since it relies solely on the collision dynamics. It is in particular transparent to the change of timescales, equation (10). However, as we argued, only the physical time is relevant to statistical averages. In this system the velocities change with the physical time and get rescaled at the periodic boundaries. The velocity dynamics of the natural time are on the other hand trivial. Thus one might wonder what happens when s is taken as the physical time, in which case we lose the connection with the Gaussian iso-kinetic dynamics. This is what we do in [14], where we discuss an expanding billiard model similar to this one, but for which the physical time dynamics is trivial between collisions and preserves phase-space volumes in the bulk. In this case, the speed variable must be rescaled at the periodic boundaries, and is associated with a third Lyapunov exponent, here negative. The mobility changes by a factor of two, and one nevertheless retrieves an identification between entropy production and phase-space contraction rates in the linear transport regime.

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