Some Estimates for 2-Dimensional Infinite and Bounded Dilute Random Lorentz Gases

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We present a (mostly) rigorous approach to unbounded and bounded (open) dilute random Lorentz gases. Relying on previous rigorous results on the dilute (Boltzmann–Grad) limit we compute the asymptotics of the Lyapunov exponent in the unbounded case. For the bounded open case in a circular region we give here an incomplete rigorous analysis which gives the asymptotics for large radius of the escape rate and of the rescaled "quasi-invariant" (q.i., or "quasi-stationary") measure. We finally give a complete proof on existence and asymptotic properties of the q.i. measure in a one-dimensional "caricature."

KEY WORDS: Lorentz gas; Boltzmann–Grad limit; Lyapunov exponents; quasistationary measures.

1. INTRODUCTION

It is well known that the statistical theory of dynamical systems (ergodic theory) was created by Boltzmann and Gibbs to address fundamental problems of kinetic theory and statistical mechanics. Much later the ideas and methods of the modern theory of dynamical systems (often refered to as less general and loosely defined chaos theory) were successfully applied to a large variety of problems in statistical mechanics and kinetic theory. Continuing these very fruitful developments, methods and approaches of kinetic theory were recently applied to estimate Lyapunov exponents,

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Kolmogorov–Sinai entropy and other dynamical characteristics for various models of gases and fluids (see refs. 1–5, and references therein).

These approaches employed both, formal and informal, versions of kinetic theory, which are based on a straightforward (geometric) analysis of the particle collisions (interactions) and on kinetic equations (dealing with expansions of their solutions), respectively.⁽⁵⁾

A rigorous approach to the derivation of the Boltzmann equation for the 2-dimensional unbounded random diluted Lorentz gas, as the Fokker– Planck–Kolmogorov equation for the Markov limiting process in the Boltzmann–Grad (BG) limit,⁽⁶⁾ was presented in ref. 7. In this paper we present a mostly rigorous approach to the analysis of unbounded and bounded (open) dilute random Lorentz gases which is mainly based on the basic ideas and constructions of ref. 7, which allow to control convergence to the limiting process for almost all configurations of the scatterers.

Here we first use the limiting process and the corresponding equilibrium distribution to compute the Lyapunov exponents for the unbounded dilute random Lorentz gas. The derivation is not entirely rigorous, the only gap being that we have to take the Boltzmann–Grad limit first, and only after that we take (macroscopic) time to infinity. The "real" Lyapunov exponents correspond instead to taking time to infinity for a fixed scatterer radius, but for random scatterers this is out of reach of the available mathematical tools.

We then study the bounded dilute random Lorentz gas with absorbing (open) boundary conditions, already in terms of the limiting process, in the particular case when the volume is a circle K_R of radius R with center at the origin. We study the eigenvalue problem for the quasi-invariant (because of the escape of particles from the region) limiting distribution. We find the asymptotics for large R of the quasi-invariant distribution and we also obtain the asymptotics of the escape rate. Such results are in good agreement with some recent physical results⁽⁸⁾ obtained with a different approach, and we plan to give a more complete analysis in a future paper. We add a complete proof about existence and asymptotic expansion of the quasi-invariant measure for a one-dimensional model with exponential jump distribution.

It is important to mention that, in contrast with the derivation of the hydrodynamic (diffusion) equation for the Lorentz gas,⁽⁹⁾ our analysis does not use the unstable manifolds (fibers) of the corresponding dynamical system. Instead one can work with any local manifolds which are transversal to (differ from) stable fibers. Indeed, the kinetic stage of the evolution of the system deals with finite times, while a hydrodynamic stage deals with very big (i.e., infinite) times. In this limit $t \to \infty$ one needs to use unstable fibers which are limits (as $t \to \infty$) of local manifolds transversal to stable

fibers. Thus the analysis of the kinetic stage of the evolution becomes somewhat easier than that of the hydrodynamic one.

For many results concerning the derivation of the limiting process and its properties we cannot report here full proofs, which would considerably increase the size of the paper, and we refer to corresponding proofs of ref. 7. We are well aware that in some cases those proofs have to be modified, and we give some indication on the necessary steps. We plan to publish in the near future an extensive paper with complete proofs.

2. BOLTZMANN-GRAD LIMIT AND LYAPUNOV EXPONENTS

We consider the Lorentz gas in the plane R^2 with random configuration of scatterers. The scatterers are circles of radius a, and the "wind" particle has unit speed, so that it is identified by a point $(q, \psi) \in M$, with $M = R^2 \times S^1$. $q = (q_1, q_2)$ are the particle coordinates and $\psi =: (\cos \psi, \sin \psi), \psi \in S^1$, is its velocity. The configuration of the scatterer centers is a point $\omega \in \Omega$, where Ω is the space of the locally finite subsets of R^2 , endowed with the topology of pointwise convergence. We take a Poisson measure on (the σ -algebra of Borel sets of) Ω with intensity measure λdq , with constant scatterer density $\lambda > 0$. So we allow the scatterers to overlap, but of course the overlapping disappears in the low density limit. One could also take other measures with fast decay of correlations, as we briefly discuss below.

The flow is just free motion with elastic collisions at the boundary of the scatterers. We repeat here the main points of the construction, which is given in detail in ref. 7.

In what follows, in order to avoid confusion, we will denote by $x \in R^2$ the scatterer centers, and by q the points of the plane accessible to the "wind" particle. Assuming that at collision times the particle has the outgoing velocity, if $D_a(x)$ denotes the (open) circle (scatterer) with center x, a particle colliding with it is represented by a point in $K_a(x) = \{(q, \psi):$ $q \in \partial D_a(x), (q-x) \cdot \psi \ge 0\}$. The part of the plane covered by the scatterers is $S_{a,\omega} = \bigcup_{x \in \omega} D_a(x)$. We need to exclude from its boundary $\partial S_{a,\omega}$ the "angular points," which belong to more than one scatterer, i.e., the set $\partial' S_{a,\omega} = \bigcup_{x,x' \in \omega, x \ne x'} \{\partial D_a(x) \cap \partial D_a(x')\}$, for which elastic reflection is not defined. The set of the admissible collision points is then

$$H_{a,\omega} = \left\{ (q,\psi) \in \bigcup_{x \in \omega} K_a(x), q \in \partial^* S_{a,\omega} \right\},\$$

with $\partial^* S_{a,\omega} = \partial S_{a,\omega} \setminus \partial' S_{a,\omega}$. What is left is the space $M_{a,\omega} = (R^2 \setminus S_{a,\omega}) \times S^1 \cup H_{a,\omega}$, from which we have to remove all points (q, ψ) such that the

trajectory, for some positive or negative t ends up at an angular point in $\partial S_{a,\omega}$. It is easy to see that this set has zero Lebesgue measure, and denoting by $M'_{a,\omega}$ the remaining set, we take it as the phase space of our system. The dynamics on $M'_{a,\omega}$ is a flow denoted $\{T^{a,\omega}_t, t \in R^1\}$, and the superscript a, ω will be often omitted.

For the BG limit it is convenient to assume the "mesoscopic picture" (see ref. 7), which allows to keep the configuration ω of the scatterer centers fixed, as we take the limit $a \rightarrow 0$. The "microscopic scale" would be the one for which the scatterer radius is fixed, and the density of the scatterers vanishes, and the "macroscopic" description, which is of main interest to us, is the one in which the free flight length is finite. As in the mesoscopic picture the free flight is of order a^{-1} , the macroscopic unit of length (and of time) is taken a^{-1} times larger than the mesoscopic one.

We introduce the discrete map $T_a^{\omega}: M'_{a,\omega} \to H_{a,\omega} \cup \overline{0}$, where $\overline{0}$ represents the absence of collision (i.e., the particle escapes at infinity). It is easy to see (see ref. 7) that the points of $M'_{a,\omega}$ which are mapped into $\overline{0}$ have zero Lebesgue measure in the unbounded case, but this is of course not true in the bounded open case. If a collision takes place, i.e., $T_a^{\omega}(q, \psi) = (q', \psi') \in H_{a,\omega}$, we denote by $\tau_a^{\omega}(q, \psi) = a |q'-q|$ the (macroscopic) length of the free path, and by $b_a^{\omega}(q, \psi) = \sin \phi \in [-1, 1]$, where ϕ is the collision angle (the angle of the outgoing velocity with the outer normal at the collision point), the impact parameter of the collision, i.e., the distance between the semiinfinite straight line starting at q in the direction ψ and the center of the scatterer with which the collision takes place, taken with positive (negative) sign if the center is on the right (left) side of the line, and divided by the scatterer radius a. By the law of elastic collision the direction of flight changes to

$$\psi' = \psi + \pi + 2 \arcsin(b_a^{\omega}) = \psi + \pi + 2\phi.$$
(1)

A point $(q, \psi) \in K_a(x)$ representing a particle colliding with the scatterer at x can be written as $(q, \psi) = (x + a\underline{\theta}, \theta + \phi)$, where $\underline{\theta} = (\cos \theta, \sin \theta)$, $\theta \in S^1$, and $\phi \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ is the collision angle. In this way $K_a(x)$ is identified with a cylinder $S^1 \times [-\frac{\pi}{2}, \frac{\pi}{2}]$. As we said in the introduction one does not need to work with the unstable manifolds, and it is enough to work with some convenient local manifolds. Such are the "increasing curves" on the cylinders $K_a(x)$ introduced in ref. 7, i.e., smooth curves $\phi(\theta)$ such that $\phi'(\theta) > 0$. It is not hard to see that increasing curves are mapped by T_a^{ω} into increasing curves, more precisely if $\gamma \subset K_a(x)$ is an increasing curve on which T_a^{ω} is continuous and $\gamma' \subset K_a(x')$ is its image, then γ' is given in terms of the coordinates (θ_1, ϕ_1) on $K_a(x')$ by the equation $\frac{d\phi_1}{d\theta_1} = 1 + \cos \phi_1(a^{-2}\tau_a^{\omega} + \frac{\cos \phi}{1+\phi'})^{-1}$, and therefore is also increasing. This is the key factor that ensures, for almost all $\omega \in \Omega$, a kind of "propagation of chaos," and convergence to the limiting Markov process.

The main result, following ref. 7, can be stated in the following terms. Let ω be fixed, and consider a bundle $\Delta_{\epsilon} = \{(q, \theta): \theta \in (\theta_* - \epsilon, \theta_* + \epsilon)\}$, assuming that $q \notin \omega$ (so that q does not belong to a scatterer for a small), and $\epsilon = \epsilon(a) > a^{\alpha}$ for some $\alpha \in [0, 1)$. Let $\mu_{\epsilon}(d\theta)$ denote the normalized Lebesgue measure on Δ_{ϵ} , and $\tau_1(\theta), \tau_2(\theta),...$ and $b_1(\theta), b_2(\theta),...$ the sequence of free flight lengths and impact parameters of the trajectories starting at q with direction θ . The following result is proved in ref. 7 for the unbounded case.

Proposition 1. For almost all $\omega \in \Omega$, the joint distribution of $\tau_1, b_1, \tau_2, b_2,...$ induced by the measure $\mu_{\epsilon}(d\theta)$ on Δ_{ϵ} tends weakly as $a \to 0$ to the limiting distribution for which all variables are independent, the variables $\{\tau_j, j = 1, 2,...\}$ are i.i.d, exponentially distributed with average $\ell = \frac{1}{2\lambda}$, and the variables $\{b_j, j = 1, 2,...\}$ are i.i.d., uniformly distributed on [-1, 1].

It is worth to spend a few words to explain the main ideas of the proof in ref. 7. The first step is based on the construction of a "good set" of configurations ω , which are, roughly speaking, those for which the joint distribution function of τ_1 and b_1 differs (in the sense of the sup norm) from the limiting distribution by a quantity that vanishes as $a \to 0$, i.e.,

$$\left\{\omega: \sup_{t>0, y\in [-1,1]} \left| \mu_{\epsilon}(\psi; \tau_{a}^{\omega}(q,\psi) \leq t, b_{a}^{\omega}(q,\psi) \leq y) - (1 - e^{-2\lambda t}) \frac{1+y}{2} \right| < a^{\eta} \right\}$$
⁽²⁾

for some conveniently small $\eta > 0$. The crucial point is that the measure of the "bad set," complement of the set above, due to the properties of the Poisson process, has a quasi-exponential decay, i.e., under the condition that there is no scatterer at a distance less than a^{β} from q, for some convenient $\beta \in (0, 1)$, the measure of the bad set vanishes as $\exp(-\kappa a^{-\delta})$, for some $\delta, \kappa > 0$. (The same would hold if, instead of the Poisson measure, we take a Gibbs state with exponential decay of correlations.) One then gets almost-sure convergence by a Borel–Cantelli argument.

The quasi-exponential decay allows to extend the result to a sufficiently dense set of bundles or more generally of "increasing curves" (growing in numbers as an inverse power of a). The Markov property is proved by showing that the images of the connected parts of the first collision map are close to the increasing curves of that set, and that the

distribution of flight length τ and impact parameter b is close to the limiting distribution.

The discrete-time limiting Markov process, with state space M, implied by Proposition 1, is easily described. Taking into account relation (1) we see that the transition measure $P(q, \psi; dq' d\psi')$ and the corresponding forward operator are given by

$$\int P(q,\psi;dq'\,d\psi')\,f(q',\theta') = \int_{S^1} d\psi'\,k(\psi-\psi')\int_0^\infty \frac{ds}{\ell}\,e^{-\frac{s}{\ell}}f(q+s\underline{\psi},\psi'),$$

where $k(\psi) = \frac{1}{4} \sin \frac{|\psi|}{2}$ is the angular kernel.

In dealing with the bounded case we consider in the mesoscopic picture the circle $K_{a^{-1}R}$ with center at the origin and radius $a^{-1}R$, and, if we want to keep $\omega \in \Omega$ fixed we assume that all scatteres outside of the circle $K_{a^{-1}R}$ are "switched off," i.e., the particle escapes by getting through them. As $a \to 0$ more and more scatterers are "switched on" by getting inside $K_{a^{-1}R}$. Denoting escape through the border of $K_{a^{-1}R}$ by the absorbing state $\bar{0}$, we have as state space for the limiting process $M_R = K_R \times S^1 \cup \bar{0}$. Convergence to the limiting process is done exactly as for the unbounded case: in fact for all finite a the transition densities of the bounded open system are the same as for the unbounded system, as long as the trajectory stays in $K_{a^{-1}R}$, and the probability of getting out of $K_{a^{-1}R}$ starting from $a^{-1}q \in K_{a^{-1}R}$ is also computed in terms of the unbounded process and has a limit $P_R(q, \psi, \bar{0})$, as $a \to 0$, by Proposition 1. It follows that the limiting discrete process for the bounded case has a transition measure P_R and a forward operator given by

$$\int_{M_{R}} P_{R}(x; dx') f(x')$$

$$= \int_{K_{R} \times S^{1}} P(q, \psi; dq' d\psi') f(q', \psi') + P_{R}(q, \psi; \bar{0}) f(\bar{0})$$

$$= \int_{S^{1}} d\psi' k(\psi - \psi') \int_{0}^{d_{R}(q, \psi)} \frac{ds}{\ell} e^{-\frac{s}{\ell}} f(q + s\underline{\psi}, \psi') + e^{-\frac{d_{R}(q, \psi)}{\ell}} f(\bar{0}).$$
(3)

Here x is the variable on M_R , and the expression of the distance $d_R(q, \psi)$ of the point q from the border in the direction ψ , adopting polar coordinates $q = r(\cos \theta, \sin \theta)$, is $d_R(q, \psi) = -r \cos(\psi - \theta) + \sqrt{R^2 - r^2 \sin^2(\psi - \theta)}$. The fact that $\bar{0}$ is absorbing is expressed by the additional relation $P_R(\bar{0}; \bar{0}) = 1$.

Going back to the dynamical system, we introduce the "stretching factor," expressing the dilation of an infinitesimal bundle of trajectories up

to the finite (macroscopic) time t. If (q, ψ) is the initial point and κ_0 is the initial curvature this is expressed by the integral (see ref. 10)

$$\lambda_a^t((q,\psi);\omega) = \frac{a}{t} \int_0^{a^{-1}t} \kappa(T_s(q,\psi)) \, ds,\tag{4}$$

where κ denotes the curvature, and is computed by the following rules. During free flight the curvature radius grows linearly in *t*, and, denoting, for short, $\kappa(s) = \kappa(T_s(q, \psi))$, if there is no collision in the time interval $(s_0, s]$ we have $\kappa(s) = \kappa(s_0)(1 + (s - s_0) \kappa(s_0))^{-1}$. At collision the curvature undergoes a jump, depending on the angle ϕ between the velocity of the particle and the outward normal of the scatterer at the collision point. Denoting by κ^- and κ^+ the curvatures before and after collision we have the well known formulas

$$\kappa_{j}^{+} = \kappa_{j}^{-} + \frac{2}{a\cos\phi_{j}} \qquad \kappa_{j}^{-} = \frac{\kappa_{j-1}^{+}}{1 + a^{-1}\tau_{j}\kappa_{j-1}^{+}}.$$
 (5)

Going over to the discrete picture, we write the stretching factor up to the *n*th (mesoscopic) collision time t_n :

$$\lambda_a^n = -\frac{a}{n} \int_0^{t_n} \kappa(T_s) \, ds = -\frac{a}{n} \left[\Lambda_a^1 + \sum_{j=1}^n \Lambda_a^j \right] \tag{6a}$$

with

$$\Lambda_a^1 = \log(1 + a^{-1}\tau_1\kappa_0), \qquad \Lambda_a^j = \log(1 + a^{-1}\tau_j\kappa_{j-1}^+), \qquad j > 1.$$
(6b)

Using relations (5) it is easy to see that the terms Λ_a^j can be written as

$$\Lambda_a^j = 2\log\frac{1}{a} + \log\left(\frac{2\tau_j}{\cos\phi_{j-1}} + a^2\xi_j\right), \qquad \xi_j = 1 + \frac{\tau_j}{\tau_{j-1}}\frac{a^{-1}\tau_{j-1}\kappa_{j-2}^+}{1 + a^{-1}\tau_{j-1}\kappa_{j-2}^+}.$$

We consider the asymptotics of this quantity for *n* fixed and $a \rightarrow 0$. We need integrability (uniform in *a*) of the quantities $\log \tau_j$ and $\log \cos \phi_j$, with respect to the distribution induced by the normalized Lebesgue mesure μ_{ϵ} on the small bundle Δ_{ϵ} (or by similar mesures on an "increasing curve") for almost all $\omega \in \Omega$. This does not follow directly from the proofs in ref. 7, but could be proved with the same methods. For instance, one would need to estimate the probability of a "bad set," analogous to the complement of the set (2), for which $|\mu_{\epsilon}(\psi: \tau_a^{\omega} > t) - e^{-2\lambda t}| > r(t) a^{\eta}$, where r(t) is a decreasing integrable function. A complete proof of such results will be published in a future paper.

Taking integrability for granted, by the Lebesgue dominated function theorem and the inequality $\log(\eta + s\xi) \leq \log(1+s) + |\log \xi - \log \eta|$, valid for all positive ξ , s, η , we get the following result.

Proposition 2. As $a \to 0$, for each fixed *n*, and almost all $\omega \in \Omega$, the following asymptotics holds

$$\lambda_{a}^{n} \sim a \left[\left(2 - \frac{1}{n} \right) \log \frac{1}{a} - \log 2 + \frac{\log \kappa_{0}}{n} + \frac{1}{n} \sum_{j=1}^{n} \log \tau_{j} - \frac{1}{n} \sum_{j=1}^{n} \log(\cos \phi_{j-1}) \right],$$
(7)

in the sense that the difference is o(a) in $L^1(\mu_{\epsilon})$.

Proposition 2 gives the Boltzmann–Grad limit of the stretching factors, for finite times, and it would not be hard to give the corresponding expression for continuous (macroscopic) times. As the limiting distribution of all quantities in the expression (7) is known, and is given by the limiting Markov process, we can proceed to compute the asymptotics for large times, by taking $n \to \infty$, which should give a kind of Lyapunov exponent in the BG limit. As all quantities τ_j and $\cos \phi_j = \sqrt{1-b_j^2}$ are independent, a simple application of the law of large numbers gives the asymptotics for large *n* in the BG limit:

$$\lambda_a^n \sim a \left[2 \log \frac{1}{a} + \log \ell + 1 - \gamma + O\left(\frac{1}{\sqrt{n}}\right) \right], \tag{8a}$$

where γ denotes the Euler constant.

Taking into account that in the limiting process the ratio $\frac{n_t}{t}$, where n_t is the number of collisions up to time t, tends to $\frac{1}{\ell}$, where ℓ is the free flight length, we find the asymptotics as $t \to \infty$ of the continuous time stretching factor (4):

$$\lambda_a^t \sim \frac{a}{\ell} \left[2 \log \frac{1}{a} + \log \ell + 1 - \gamma + O\left(\frac{1}{\sqrt{n}}\right) \right]. \tag{8b}$$

This expression coincides with the asymptotics found in ref. 11 for the Lyapunov exponent of the periodic Lorentz gas in the limit as the scatter radius vanishes, an indication that, in spite of the fact that we have inverted the limiting procedures, by taking first $a \rightarrow 0$ and then $t \rightarrow \infty$, the expression (8b) gives the correct asymptotics of the Lyapunov exponents of the Lorentz gas with random scatterers.

3. QUASI-STATIONARY MEASURES FOR THE BOUNDED OPEN CASE

We now consider the discrete-time limiting process in the circle K_R with forward operator given by Eq. (3). Mass is lost across the border (represented by the absorbing state $\overline{0}$), so that there is no positive invariant probability measure. It is however to be expected that, starting with some initial "nice" probability measure, as time goes on, a kind of stationary regime sets in, in the sense that if one considers the sequence of probability measures obtained by applying the evolution operator, under the condition that the process has not been absorbed (i.e., dividing by the total mass that is left), one gets to a quasi-stationary measure which is invariant under such procedure.

Unfortunately we do not know of any results on existence, uniqueness and convergence to the limiting distribution that can be applied to our case. Rigorous results up to now have been proved only for the case of discrete state space (see, e.g., ref. 12). In such cases it can be seen that a condition for existence is "exponential absorption," i.e., if T is the absorption time, then for some $\lambda > 0$ the conditional expectation of $e^{\lambda T}$ under the condition that x is the starting point, is finite, i.e., $E_x e^{\lambda T} < \infty$, for all x. This is certainly true in our case, and we hope to be able to prove rigorous results in the future. What we can do now is to write down the eigenvalue equation for the quasi-invariant (q.i.) measure, and, under some appropriate assumptions, find out some properties of the solution.

We are mainly interested in knowing how the asymptotics of the stretching factor is modified in the finite open case. It is clear that the discrete-time stretching factor will always be given by the expression (7), but the continuous time stretching factor will differ from expression (8b), because the mean free path will not be equal to ℓ , but is replaced by an average on the quasi-stationary measure, and will be smaller. We consider the case of a circle K_R of radius R, and, under some reasonable assumptions, we find the asymptotic behavior of the escape rate (logarithm of the fraction of mass that escapes) and of the quasi-invariant (*R*-rescaled) measure for large R. In order to compute the correction to the free flight length we would need however the corrections of order $\frac{1}{R}$ to the limiting quasi-invariant measure, which is again the object of further work.

At the end of the section we will show how one can give a rigorous solution to the problem of finding out the asymptotics of the quasi-stationary measure in a 1-dimensional model.

We go back to the process with forward operator given by Eq. (3), and look for a quasi-stationary probability measure with smooth density $f(q, \psi)$. It is natural to assume that the solution belongs to the class V of

the rotation invariant functions, i.e., of the functions that, going over to polar coordinates $q = r(\cos \theta, \sin \theta)$ depend on r and $\cos(\psi - \theta)$ only. Both the operator in (3) and the corresponding backward operator map the class V into itself. If $\beta(R)$ is the total mass that is left in M_R , we see that the equation for the quasi-stationary measure is

$$\int_{S^1} k(\psi - \psi') \, d\psi' \int \frac{ds}{\ell} e^{-\frac{s}{\ell}} f(q - s\underline{\psi}', \psi') \, \chi_{K_R}(q - s\underline{\psi}') = \beta(R) \, f(q, \psi), \quad (9a)$$

where χ_{K_R} denotes the indicator function. $\beta(R)$ is connected to the continuous-time escape rate which is used in the physical literature. We prefer a discrete-time formulation which leads to a mathematically well defined eigenvalue problem.

Consider the space Fourier transform $\hat{f}(\lambda, \psi) = \int_{K_R} e^{i(\lambda, q)} f(q, \psi) dq$. As $f \in V$ we write from now on $f(r, \cos(\psi - \theta))$, and the Fourier transform \hat{f} is also a function in V, which, in polar coordinates $\lambda = |\lambda| (\cos \theta, \sin \theta)$, can be written as $\hat{f}(|\lambda|, \cos(\psi - \theta))$. After some tedious calculations, setting $l = |\lambda|$, we see that \hat{f} satisfies the following eigenvalue equation

$$\int_{S^1} k(\psi - \psi') g(l, \cos \psi') \hat{f}(l, \cos \psi') d\psi' - S(l, \psi) = \beta(R) \hat{f}(l, \cos \psi),$$
(9b)

where $g(l, \cos u) = \frac{1}{1 - i\ell l \cos u}$ comes from the transition kernel. The function S needs some accurate computation. Expressing λ in polar coordinates and setting $\hat{\psi} = \psi - \theta$, $D(r) = \frac{e^{-r/\ell}}{\ell r}$, we have

$$S(|\lambda|, \hat{\psi}) = \int_{K_R^c} dy \, e^{i(\lambda, y)} \int_{K_R} dx \, k(\theta - \arg(y - x)) \, D(|y - x|) \, f(x, \arg(y - x))$$
$$= \int_R^\infty \rho \, d\rho \int du \, e^{i \, |\lambda| \, \rho \cos u}$$
$$\times \int_0^R r \, dr \int d\phi \, k(\hat{\psi} - u - w(\phi)) \, D(\rho, r, \phi) \, f(r, \cos w_*(\phi)).$$

Here the new variables are: u is the anomaly of y, ϕ is the angle between y and x, $w_*(\phi)$ is the angle between y-x and x, and $w(\phi) = w_*(\phi) - \phi$. Taking into account that

$$\int du \, k(\theta - u) \, e^{ia\cos u} = J_0(a) + 2 \sum_{k=1}^{\infty} i^k \lambda_k J_k(a) \cos k\theta$$

where the functions $\{\cos k\theta\}_{k=0}^{\infty}$ are eigenfunctions of the angular operator with kernel $k(\cdot)$, $\lambda_k = (1-4k^2)^{-1}$ the corresponding eigenvalues, and J_k are the Bessel functions, we get the Fourier expansion $S(l, \theta) = \sum_{k=0}^{\infty} i^k S_k(l) \times \cos k\theta$ where

$$S_{0}(l) = \int_{R}^{\infty} \rho \, d\rho \, m_{R}^{(0)}(\rho) \, J_{0}(l\rho), \qquad S_{k}(l) = 2\lambda_{k} \int_{R}^{\infty} \rho \, d\rho \, m_{R}^{(k)}(\rho) \, J_{k}(l\rho),$$
(10)
$$m_{R}^{(k)}(\rho) = \int_{0}^{R} r \, dr \int d\phi \, D(\rho, r, \phi) \cos[kw(\phi)] \, f(r, \cos[w_{*}(\phi)]).$$

Introducing the Fourier expansion for $f: f(r, \cos \psi) = \sum_{k=0}^{\infty} f_k(r) \cos k\psi$, we find for \hat{f}

$$\hat{f}(l,\cos\psi) = \sum_{j=1}^{\infty} i^k \hat{f}_k(l) \cos k\psi, \quad \hat{f}_k(l) = 2\pi \int_0^R r \, dr \, f_k(r) \, J_k(lr).$$
(11a)

The expansion for $g(l, \cos \psi)$ is

$$g(l,\cos\psi) = \sum_{j=1}^{\infty} (-il\ell)^k g_k(l\ell) \cos k\psi, \qquad (11b)$$

where it can be seen that $g_k(0) = 1$. Observe that the first component of g is the Fourier transform of the averaged (over angles) transition probability:

$$g_0(|\lambda|) = \frac{1}{2\pi} \int \frac{d\theta}{1 + \ell^2 |\lambda|^2 \cos^2 \theta} = \frac{1}{2\pi} \int_{R^2} e^{i(\lambda, x)} \frac{e^{-\frac{|\lambda|}{\ell}}}{\ell |x|} dx = \frac{1}{\sqrt{1 + \ell^2 |\lambda|^2}}$$

Taking into account that all components S_k and \hat{f}_k vanish for l = 0 if k > 0, and that the normalization condition for the measure gives $\hat{f}_0(0) = \frac{1}{2\pi}$ we find that

$$1 - \beta(R) = 2\pi S_0(0) = 2\pi \int_R^\infty \rho \, d\rho \, m_R^{(0)}(\rho). \tag{12}$$

Inserting the Fourier expansions in the main equation (9b) we get a sequence of equations for the components $\hat{f}_k(l)$, which are coupled, due to the integral term. From now on we consider the rescaled density $f^{(R)}(x, \psi) = R^2 f(Rx, \psi)$, which is defined in the unit circle $x \in K_1$, in the asymptotic regime of large R. The Fourier transform of $f^{(R)}$ is $\hat{f}^{(R)}(\lambda, \psi) = \hat{f}(\frac{\lambda}{R}, \psi)$, and we have just to replace λ by $\frac{\lambda}{R}$ in Eq. (9b). We first write the

components of $S_k(\frac{l}{R})$ in a convenient way. Observe that, for all $k \ge 0$, $|m_R^{(k)}(\rho)| \le m_R^{(0)}(\rho)$, and using the normalization condition (12) we see that

$$\frac{2\pi}{1-\beta(R)}\int_{R}^{\infty}\rho\,d\rho\,m_{R}^{(k)}(\rho)\,J_{k}\left(\frac{\rho l}{R}\right)=\gamma_{k}J_{k}\left(l\left(1+\frac{s_{k}}{R}\right)\right),$$

where $|\gamma_k| \leq 1$, and, by the property of rapid decay of the density measure for large $\rho - R$, due to the exponential factor $D(\rho, r, \phi)$, one can assume (and will have to prove in a rigorous analysis) that the quantities s_k stay bounded as R grows, no matter what the unknown density $f^{(R)}$ (which appears in $m_R^{(0)}(\rho)$) is.

Setting $\lambda_k^* = -\lambda_k > 0$ for k > 0 we see that Eq. (9b) is equivalent to the following system of infinite coupled equations

$$2\pi \int d\psi \ g\left(\frac{l}{R}, \cos\psi\right) \hat{f}^{(R)}(l, \cos\psi) - \beta(R) \ \hat{f}_{0}^{(R)}(l)$$
$$= (1 - \beta(R)) \ J_{0}\left(l\left(1 + \frac{s_{0}}{R}\right)\right)$$
$$\int d\psi \cos k\psi g\left(\frac{l}{R}, \cos\psi\right) \hat{f}^{(R)}(l, \cos\psi) + \frac{\beta(R)}{\lambda_{k}^{*}} \ \hat{f}_{k}^{(R)}(l)$$
$$= (1 - \beta(R)) \ \gamma_{k}^{*} \ J_{k}\left(l\left(1 + \frac{s_{k}}{R}\right)\right), \qquad k > 0,$$

where, according to the assumptions above, the numbers γ_k^* and s_k are bounded, for bounded *l*, uniformly in *R*. The expansion (11b), with *l* replaced by $\frac{l}{R}$, when inserted in (9b) allows to express the left sides of the equations above as a sum of contributions of different orders in R^{-1} . We write down the first two:

$$2\pi \left(\left(g_0 \left(\frac{l}{R} \right) - \beta(R) \right) \hat{f}_0^{(R)}(l) + \frac{\ell l}{2R} g_1 \left(\frac{l}{R} \right) \hat{f}_1^{(R)}(l) + \frac{\ell^2 l^2}{2R^2} g_2 \left(\frac{l}{R} \right) \hat{f}_2^{(R)}(l) + \cdots \right)$$

$$= (1 - \beta(R)) J_0 \left(l \left(1 + \frac{s_0}{R} \right) \right)$$

$$(13a)$$

$$\hat{f}_1^{(R)}(l) \left(g_0 \left(\frac{l}{R} \right) + \frac{\beta(R)}{\lambda_1^*} \right) + \frac{\ell l}{R} g_1 \left(\frac{l}{R} \right) \left(\frac{\hat{f}_2^{(R)}(l)}{2} - \hat{f}_0^{(R)}(l) \right)$$

$$+ \frac{\ell^2 l^2}{R^2} g_2 \left(\frac{l}{R} \right) (\hat{f}_3^{(R)}(l) - \hat{f}_1^{(R)}(l)) + \cdots$$

$$= (1 - \beta(R)) \gamma_1^* J_1 \left(l \left(1 + \frac{s_1}{R} \right) \right).$$

$$(13b)$$

The left hand side of the equations for k > 1 has the same structure as (13b), and it would not be hard to give the general form. In particular they start with a term $\hat{f}_{k}^{(R)}(l)(g_{0}(\frac{l}{R}) + \frac{\beta(R)}{\lambda_{k}^{*}})$, which should be of the same order as the right term, which is $(1 - \beta(R))$ times a function that is bounded for bounded *l*, uniformly in *R*. As $g_{0} > 0$, the eigenvalue $\beta(R) \rightarrow 1$ for large *R*, and $\lambda_{k}^{*} > 1$, $\hat{f}_{k}^{(R)}(l)$ should be at least of the same order of smallness as $1 - \beta(R)$.

On the basis of such analysis one can see that a consistent scaling limit exists with $1-\beta(R) \sim \frac{\kappa}{R^2}$, $\hat{f}_0^{(R)}(\ell) \sim \bar{f}_0(\ell)$, $\hat{f}_1^{(R)}(\ell) \sim \frac{1}{R} \bar{f}_1(\ell)$, and $\hat{f}_k^{(R)}(\ell) \sim \frac{1}{R^2} \bar{f}_k(\ell)$ for k > 1. Substituting into Eq. (13b), setting $\bar{f}_1^{(R)}(l) = R \hat{f}_1^{(R)}(l)$, taking into account that $\lambda_1^* = \frac{1}{3}$ we get, as $R \to \infty$, the relation

$$\bar{f}_{1}^{(R)}(l)\left(g_{0}\left(\frac{l}{R}\right)+3\beta(R)\right)-l\ell g_{1}\left(\frac{l}{R}\right)\hat{f}_{0}^{(R)}(l)=O\left(\frac{1}{R}\right).$$
(14)

Taking the limit as $R \to \infty$ we obtain for the limiting functions the equality $\bar{f}_1(l) = \frac{l\ell}{4} \bar{f}_0(l)$. Plugging Eq. (14) into Eq. (13a), we see after some simple manipulations that

$$2\pi \left(g_0 l \left(\frac{l}{R} \right) - \beta(R) + \frac{l^2 \ell^2}{8R^2} \right) \hat{f}_0^{(R)}(l) + O\left(\frac{1}{R^3} \right)$$
$$= (1 - \beta(R)) J_0 \left(l \left(1 + \frac{s_0}{R} \right) \right). \tag{15}$$

As s_0 is positive and bounded, it is easily seen that the Bessel function on the right, which starts with positive values for small l, has a simple zero at some point $l_* < \xi_1$, $l_* = \xi_1 + O(\frac{1}{R})$, where ξ_1 is the first zero of J_0 . As we are looking for a nondegenerate asymptotic solution that is not concentrated on the border of K_1 , we can safely assume that $\hat{f}_0^{(R)}(l)$ is positive and uniformly (in R) bounded away from 0 in a neighborhood of ξ_1 . Hence, by a simple computation, taking into account that $1 - g_0(\frac{1}{R}) \sim \frac{\ell^2 l^2}{2R^2}$, we find

$$1 - \beta(R) = \frac{3\xi_1^2 \ell^2}{8R^2} \left(1 + O\left(\frac{1}{R}\right) \right).$$
(16)

Going back to Eq. (15) we find the asymptotics of the first two components $\hat{f}_{0}^{(R)}$ and $\hat{f}_{1}^{(R)}$ of the asymptotic quasi-stationary measure:

$$\lim_{R \to \infty} \hat{f}_0^{(R)}(l) = \frac{1}{2\pi} \frac{J_0(l)}{1 - \frac{l^2}{\xi_1^2}}, \qquad \hat{f}_1^{(R)}(l) \sim \frac{l\ell}{8\pi R} \frac{J_0(l)}{1 - \frac{l^2}{\xi_1^2}}.$$
 (17)

This result implies that the rescaled measure $f^{(R)}(x, \psi)$ has a limit as $R \to \infty$ which is of the type $NJ_0(\xi_1 |x|)$, where N is a normalization constant. Relations (17) are however not enough to compute the corrections of order $\frac{1}{R}$ to the average free flight, as one would need the corrections of order $\frac{1}{R}$ to the asymptotics of $f_0^{(R)}(l)$, and this could be done only by getting more information on the asymptotic behavior of the quantity s_0 appearing in Eq. (13a). This is, as we said, a task for future work.

The asymptotic expansion of the escape rate given by Eq. (16) is in agreement with the results of ref. 8, obtained with a completely different approach, based on the analysis of an "extended Lorentz–Boltzmann equation." In terms of the physical quantities introduced in that paper, relation (16) can be reformulated by saying that the (continuous time) escape rate is $\gamma = \frac{1-\beta}{\ell} = D\xi_1^2\ell$, where D is interpreted as the diffusion coefficient. We are not able however to compare with the higher order expansion of the density function obtained in ref. 8, and in particular we cannot say anything at the present stage about the contribution of boundary layer terms to higher orders.

We conclude this section by showing how, by applying the main ideas of the procedure sketched above, one can give a rigorous solution to the problem of finding the needed asymptotics of the quasi-stationary measure in a one-dimensional caricature.

Consider the discrete process on R with symmetric exponential jump distribution $p(x) = \frac{1}{2\ell} e^{-\frac{|x|}{\ell}}$, where ℓ is the free flight length. We consider the equation for the quasi-stationary measure in an interval $I_R = [-R, R]$, the density of which is denoted by f, normalized as $\int_{-R}^{R} f(x) dx = 1$. The equation is

$$(P^*f)(x) = \int_{-R}^{R} f(y) \, p(x-y) \, dy = \beta(R) \, f(x), \qquad x \in [-R, R].$$
(18)

The following theorem holds.

Theorem 1. For all *R* there is a unique positive solution $f \in L^2[-R, R]$ of the eigenvalue problem (18) with maximal positive eigenvalue $\beta(R)$. Moreover *f* is differentiable, and the following asymptotics holds as $R \to \infty$ for the eigenvalue $\beta(R)$ and the rescaled eigenfunction $f^{(R)}(x) = Rf(Rx), x \in [-1, 1]$

$$1 - \beta(R) = \frac{\pi^2 \ell^2}{4R^2} \left(1 + O\left(\frac{1}{R}\right) \right)$$
(19a)

$$f^{(R)}(x) = \frac{\pi}{4} \cos\frac{\pi x}{2} + \frac{\pi \ell}{4R} \left(\frac{\pi x}{2} \sin\frac{\pi x}{2} - \cos\frac{\pi x}{2}\right) + O\left(\frac{1}{R^2}\right).$$
(19b)

Proof. The fact that there is a unique positive eigenfunction in $L^2[-R, R]$ with maximal positive eigenvalue follows from classical theorems (see ref. 13, Section 7). As the kernel is a.s. differentiable with bounded derivative, so is f. Moreover, as the integration kernel leaves the subspaces of the even (in x) and odd functions invariant, f has to be even.

Going over to the Fourier transform $\hat{f}(\lambda) = \int_{I_R} e^{i\lambda x} f(x) dx$, Eq. (18) becomes

$$\beta(R) \ \hat{f}(\lambda) = \tilde{p}(\lambda) \ \hat{f}(\lambda) - \int_0^\infty A_R(s) \cos(\lambda(R+s)) \ ds, \qquad (20a)$$

where $\tilde{p}(\lambda) = \frac{1}{1+\lambda^2 \ell^2}$ is the Fourier transform of the jump distribution p(x), and

$$A_R(s) = \int_0^{2R} dv f(R-v) p_+(v+s), \qquad p_+(s) = \frac{1}{\ell} e^{-\frac{s}{\ell}}, \qquad s > 0.$$

 A_R is the density of the mass that gets out and p_+ is the one-sided jump distribution. Taking $\lambda = 0$ in Eq. (20a) we get the relation

$$1 - \beta(R) = \int_0^\infty A_R(s) \, ds = \int_0^{2R} dv \, f(R - v) \, e^{-\frac{v}{\ell}}$$

expressing the fact that the total mass getting out of I_R is $1 - \beta(R)$. For the normalized density we find that $a_R(s) = \frac{A_R(s)}{1 - \beta(R)} = p_+(s)$, and we see that it does not depend on f.

Going over to the rescaled density, which has Fourier transform $\hat{f}^{(R)}(\lambda) = \hat{f}(\frac{\lambda}{R})$, Eq. (20a) becomes

$$\hat{f}^{(R)}(\lambda)\left(\tilde{p}\left(\frac{\lambda}{R}\right) - \beta(R)\right) = (1 - \beta(R))\int_0^\infty \cos\left(\lambda\left(1 + \frac{s}{R}\right)\right)\frac{1}{\ell}e^{-\frac{s}{\ell}}ds.$$
 (20b)

Introducing the Fourier transform $\tilde{p}_*(\lambda) = \frac{1}{1-\ell\lambda}$ of p_+ , we see that the integral on the right side can be written as

$$\operatorname{Re}\left[e^{i\lambda}\tilde{p}_{+}\left(\frac{\lambda}{R}\right)\right] = \frac{\cos\lambda - \frac{\lambda\ell}{R}\sin\lambda}{1 + \frac{\lambda^{2}\ell^{2}}{R^{2}}},$$

which vanishes if $\lambda = \lambda_*$, where λ_* is a solution of the equation $\cos \lambda = \frac{\lambda \ell}{R} \sin \lambda$. A simple calculation shows that for large *R* we have $\lambda_* = \frac{\pi}{2(1+\frac{\ell}{R})} + O(\frac{1}{R^3})$. As $\hat{f}^{(R)}(\lambda)$ cannot vanish for $\lambda < \frac{\pi}{2}$ we see that $\beta(R) = \tilde{p}(\frac{\lambda_*}{R})$, which gives immediately the asymptotics (19a).

Equation (20b) can now be solved for $\hat{f}^{(R)}(\lambda)$, which turns out to be

$$\hat{f}^{(R)}(\lambda) = \frac{\lambda_*^2}{\lambda_*^2 - \lambda^2} \left(\cos \lambda - \frac{\lambda \ell}{R} \sin \lambda \right).$$
(21a)

The inverse Fourier transform can be computed as a residue integral, and gives

$$f^{(R)}(x) = \frac{\lambda_* \sin \lambda_*}{2} \left(1 + \frac{\ell^2 \lambda_*^2}{R^2} \right) \cos \lambda_* x, \qquad |x| \le 1,$$
(21b)

and, of course, $f^{(R)}(x) = 0$ is |x| > 1. By expanding λ_* in inverse powers of R we get the asymptotics (19b).

Theorem 1 is proved.

It is worth to remark that the quasi-stationary density (21b) is discontinuous at the border points $x = \pm 1$, where it has a jump of order $\frac{1}{R}$, more precisely it can be seen that $f^{(R)}(\pm 1) = \frac{\pi^2 \ell}{8R} + O(\frac{1}{R^2})$.

Note that the asymptotic behavior of the measure, as for the Lorentz gas, has a leading term that does not depend on the particular distribution (i.e., in this case, on ℓ), whereas the correction of order $\frac{1}{R}$ depends on it. This seems to be a general fact.

In the 1-dimensional case, if the distribution is not exponential, the problem is more complicated, as one has to investigate the asymptotic properties of the measure $a_R(s)$, which would depend on the density f itself.

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REFERENCES

- H. van Beijeren and J. R. Dorfman, Lyapunov exponents and Kolmogorov-Sinai entropy for the Lorentz gas at low densities, *Phys. Rev. Lett.* 74:4412–4415 (1995); Erratum: *ibid.* 76:3238 (1996).
- H. van Beijeren, J. R. Dorfman, H. A. Posch, and Ch. Dellago, Kolmogorov–Sinai entropy for dilute gases in equilibrium, *Phys. Rev. E* 56:5272–5277 (1997).
- 3. P. Gaspard, *Chaos, Scattering and Statistical Mechanics* (Cambridge University Press, 1998).
- R. Dorfman, An Introduction to Chaos in Nonequilibrium Statistical Mechanics (Cambridge University Press, 1999).

- R. van Zon, H. van Beijeren, and J. R. Dorfman, Kinetic theory estimates for the Kolmogorov–Sinai entropy, and the largest Lyapunov exponents for dilute, hard ball gases and for dilute, random Lorentz gases, in *Hard Ball Systems and the Lorentz Gas*, D. Szasz, ed. (Springer, 2000).
- H. Grad, Principles of the Kinetic Theory of Gases, in *Handbuch der Physik*, Vol. 12, S. Fluegge, ed. (Springer, 1958).
- C. Boldrighini, L. A. Bunimovich, and Ya. G. Sinai, On the Boltzmann equation for the Lorentz gas, J. Stat. Phys. 32:477–501 (1983).
- H. van Beijeren, A. Latz, and J. R. Dorfman, Chaotic Properties of dilute two- and threedimensional random Lorentz gases, II. Open systems, *Phys. Rev. E* (2000).
- L. A. Bunimovich and Ya. G. Sinai, Statistical properties of Lorentz gas with periodic configuration of scatterers, *Comm. Math. Phys.* 78:479–497 (1981).
- Ya. G. Sinai, Dynamical systems with elastic collisions, *Russ. Math. Surv.* 25:137–189 (1970).
- N. I. Chernov, A new proof of the Sinai formula for computing the entropy of hyperbolic billiards. Application to a Lorentz gas and to the Bunimovich stadium. (Russian) *Funktsional. Anal. i Prilozhen.* 25:50–69, 95 (1991), translation in *Funct. Anal. Appl.* 25 (1991), no. 3, 204–219 (1992).
- P. A. Ferrari, H. Kesten, S. Martinez, and P. Picco, Existence of quasi-stationary distributions. A renewal dynamical approach, *Ann. Probab.* 23(2):501–521 (1995).
- M. G. Krein and M. A. Rutman, *Linear Operators Leaving Invariant a Cone in a Banach Space*, Amer. Math. Soc. Translation 1950, No. 26 (1950), 128 pp.