Dispersion of particles in an infinite-horizon Lorentz gas

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We consider a two-dimensional Lorentz gas with infinite horizon. This paradigmatic model consists of pointlike particles undergoing elastic collisions with fixed scatterers arranged on a periodic lattice. It was rigorously shown that when \( t \to \infty \), the distribution of particles is Gaussian. However, the convergence to this limit is ultralow, hence it is practically unattainable. Here, we obtain an analytical solution for the Lorentz gas’ kinetics on physically relevant timescales, and find that the density in its far tails decays as a universal power law of exponent \(-3\). We also show that the arrangement of scatterers is imprinted in the shape of the distribution.

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The Lorentz gas (LG) is a classical model of transport [1,2], in which a pointlike particle moves at a constant speed, while undergoing elastic collisions with fixed scatterers [1–17]. When the free paths in this model are unbounded, it is termed the infinite-horizon LG (see Ref. [18] for a review). Originally suggested as a description for the movement of electrons through a conductor, it is one of the first deterministic models to show a superdiffusive behavior, and as such it plays an important role in studying diffusion phenomena. Beautiful properties of the transport and ergodicity of the infinite-horizon LG were thoroughly investigated by mathematicians. For the two-dimensional case, Bleher [19] showed that \( \lim_{t \to \infty} [r(t) - r(0)]/\sqrt{\ln(t)} \) is a Gaussian variable, where \( r(t) \) is the particle’s position at time \( t \). However, this limit theorem hides the physically observable nature of the process [19,20], as it is valid only when \( \ln[\ln(N)]/\ln(N) = \epsilon < 1 \), where \( N \) is the number of collisions. Thus, even if \( N \) is very large, this condition cannot be satisfied (e.g., \( \epsilon = 0.01 \Rightarrow N \approx 10^{281} \)). In addition, as noted by Dettmann [18], the variance of this Gaussian limiting law is half of the mean-square displacement, which suggests that the far tails of the expanding packet deviate from a Gaussian.

In this Rapid Communication, we present a theory which captures the kinetics of the packet’s density on physically attainable timescales and describes correctly its tails. By employing the Lévy walk (LW) formalism, we go beyond the Gaussian description and use what we call a Lambert scaling approach, which converges already when \( \theta = 0 \), the number of collisions. Thus, even if \( N \) is very large, this condition cannot be satisfied (e.g., \( \epsilon = 0.01 \Rightarrow N \approx 10^{281} \)). In addition, as noted by Dettmann [18], the variance of this Gaussian limiting law is half of the mean-square displacement, which suggests that the far tails of the expanding packet deviate from a Gaussian.

Fat-tailed traveling times. In an infinite-horizon LG, a particle’s trajectory exhibits intermittency. Namely, the particle undergoes epochs of diffusivelike behavior with many random reorientations, after which it follows an almost ballistic path within the endless corridors [see Fig. 1(b)]. This behavior leads to long travel times \( \tau_n \) between collision events, for which the probability density function (PDF) of \( \tau \) follows a fat-tailed law [21,22], such that its variance diverges just marginally,

\[
\lim_{t \to \infty} \tau^3 \psi(t) = \tau_0^2.
\]

Importantly, Eq. (1) is valid for spatial dimensions \( d < 6 \) [18]. The displacement of the particle is \( r(t) - r(0) = \sum_{n=1}^{N} v_n \tau_n + v_t \tau^* \). Here, \( N \) is the random number of collisions until time \( t \), \( \tau_n \) is the walking time of the \( n \)th travel epoch, \( v_n \) with \( n \geq 1 \) is the velocity just after the \( n \)th collision, \( v_t \) and \( r(0) \) are the initial velocity and displacement which are both randomly chosen, and the last traveling event is of duration \( \tau^* = t - \sum_{n=1}^{N} \tau_n \). During this process the particle’s speed is fixed due to the collisions’ elasticity, and we choose \( V = |v_t| = 1 \). Our key assumption is that the LG model, being a chaotic system, can be described as a renewal process. This means we assume no correlation between two adjacent velocities.

Using the renewal assumption, we apply the LW approach [23–25] to the LG model. We define a process where the flight times \( \tau_n \) are independent identically distributed random variables drawn from the fat-tailed PDF, Eq. (1). Similarly, the velocities \( v_n \) after each collision are drawn from a PDF we denote \( F(v) \). A simple geometrical calculation shows that for the chosen range of radii, one has a couple of perpendicular open horizons stretching to infinity, creating a crosslike density profile (see Fig. 2). Decreasing the radius opens more horizons and results in more complex shapes (for example, when \( 1/\sqrt{2} < R < 1/\sqrt{3} \), one finds that infinite corridors transport particles via the main diagonals as well [18,20], yielding a Union Jack flag geometry). Out of this consideration, we use a velocity PDF which is aligned along the lattice’s axes, and since the speed is set to one, we have \( F(v) = [\delta(v - 1) + \delta(v + 1)]\delta(v_x) + \delta(v_y)\delta(v_x)\delta(v_y) - 1 + \delta(v_y + 1)]/4 \). The
renewal assumption basically identifies the flight times’ PDF of the LW approach with that of the LG model, and we obtain the latter.

Therefore, we devise a method to calculate the cumulative distribution function (CDF) of the walking times of the LG, CDF(τ) = ∫_0^τ dτ′ψ(τ′), which was previously studied in the limit R/a → 0 [26]. The CDF is obtained from geometrical considerations and the ergodic property of the underlying process. Starting from a given scattering event, we calculate the distance to the next scatterer, and since the particles travel with unit speed, this is also the time elapsed until the next collision. This time duration is controlled by two parameters, the angle of traveling direction and the initial impact parameter, so the small-angle approximation basically identifies the flight times’ PDF with the ergodic property of the dynamics implies that the distributions of these parameters are both uniform [28]. We then average over all possible time durations with respect to the aforementioned parameters, thus finding an analytical expression for the traveling times’ CDF. This function, which is a key ingredient for the theory presented below, exhibits rich behaviors, for example, oscillations due to the discrete nature of the scatterers’ lattice arrangement [see Fig. 1(c)]. Asymptotically, we get the known long-time limit law of ψ(τ) ∝ τ^-3, for which the original proof is valid in the limit R → a/2 [21], when the oscillations are damped out.

The solution. Let P(r,t) be the density of particles, all starting at r(0) = 0, and denote Π(k,u) as its Fourier-Laplace transform, r → k,t → u. An exact solution for Π(k,u) is given by the familiar Montroll-Weiss equation [24]

Π(k,u) = \left( \frac{1 - \hat{\psi}(u - ik \cdot v)}{u - ik \cdot v} \right) \frac{1}{1 - \langle \psi(u - ik \cdot v) \rangle},

(2)

where \hat{\psi}(u) is the Laplace transform of ψ(τ), and the ⟨···⟩ above denotes an average with respect to the velocity’s PDF F(v). To invert this equation in the long-time limit [29], we consider the small u behavior of \hat{\psi}(u), derived in the SM [27],

\hat{\psi}(u) \simeq 1 - \langle \tau \rangle u - \frac{1}{2}(\tau_0 u)^2 \ln(C_\psi \tau_0 u) + o(u^2).

(3)

FIG. 2. The probability density functions of a numerical simulation of the Lorentz gas with two open horizons (a) and the Lévy walk (LW) theory (b) for duration t = 10^4. The non-Gaussian crosslike shape clearly illustrates the sensitivity of the spreading density to the underlying structure of the square lattice of scatterers. The LW approximation Eq. (5) is in agreement with the simulation without any fitting. Further details can be found in the Supplemental Material [27].
The first term is the normalization, \( \langle \tau \rangle \) is the mean time between collisions, and the last term is related to the power-law tail of \( \psi(\tau) \), with \( C_\psi \) being

\[
C_\psi = \exp \left\{ \frac{\gamma - 3}{2} - \int_0^{\tau_0} d\tau \frac{\psi(\tau)}{\tau^2} \right\} - \int_{\tau_0}^\infty d\tau \left[ \frac{\psi(\tau)}{\tau^2} - \frac{1}{\tau} \right],
\]

where \( \gamma \approx 0.5772 \) is Euler’s constant. Importantly, we obtain the parameters \( \langle \tau \rangle, \tau_0 \), and \( C_\psi \) out of the geometrical theory of CDF(\( \tau \)). The packet of spreading particles in the long-time limit is found with an asymptotic small \( \{k, n\} \) expansion of Eq. (2), performed in the SM [27],

\[
P(r, t) \simeq \frac{1}{\pi} \frac{r^2}{\xi^2(t)} \exp \left\{ - \frac{r^2}{\xi^2(t)} \right\}
\times \left\{ 1 + \frac{1}{\Omega(t)} \sum_{j=1}^2 \left[ \frac{2 - \gamma - \ln(4)}{2} - \frac{r_j^2}{\xi^2(t)} \right] \right\}^{-\frac{1}{2}} M^{(1,0)}(1; 1: 1; 3),
\]

where

\[
\xi(t) = \frac{1}{\sqrt{\frac{2\pi}{1}}}, \quad \Xi = 2C_\psi \tau_0 V,
\]

\[
\Omega(t) = W_{-1}\left( -\frac{2T}{t} \right), \quad T = 4C_\psi^2 \langle \tau \rangle,
\]

with \( r = (r_1, r_2) = (x, y) \), and, as mentioned, \( V = 1 \). Here, \( M^{(\cdot \cdot \cdot)} = \text{Kummer’s confluent hypergeometric function} [30] \), and the superscript over \( M \) denotes the derivative with respect to its first argument. \( W_{-1}(\eta) \) is the secondary branch of the Lambert W function [30], defined for \( \eta \in [-1/e, 0] \) by the identity \( W_{-1}(\eta) = \ln(\eta/W_{-1}(\eta)) \), which has the following expansion as \( \eta \to 0^+ \),

\[
W_{-1}(\eta) = L_1 + L_2 + \frac{L_3}{L_1} + O\left( \frac{L_2^2}{L_1^2} \right).
\]

As shown in Figs. 2 and 3, the solution Eq. (5) perfectly matches the simulations without any fitting, and it nicely captures the three main features of our analysis: (I) The underlying symmetry of the scatterers is reflected in the crosslike shape of the packet of particles, (II) the longstanding problem of the ultraslow convergence is solved (see below), and (III) a power-law decay of the distribution along the open horizons.

By virtue of Eqs. (6) and (7), we have \( \Omega(t) \simeq \ln(t) \) when \( t \to \infty \), and thus the displacement \( |r| \) scales as \( \sqrt{\ln(t)} \), as was shown in Ref. [19]. However, considering the correction to this leading order, \( L_2 \) in Eq. (7), we see that one needs to demand that \( \ln(t) \gg \ln[\ln(t)] \), and as such the convergence to this mathematical limit is ultraslow. The Lambert scaling approach resolves this problem for any reasonably large \( t \), namely, time for which \( \Omega(t) \gg 1 \), by compactly enclosing all of the \( t \)-dependent logarithmic behaviors into a single function, i.e., the Lambert W function. This also means that our theory can be regarded as a series expansion in powers of a single large parameter \( \Omega(t) \), in contrast with a nested variety of logarithmic expressions which one would receive by using the standard \( \ln(\ln(t)) \) scaling in a perturbative expansion, as Eq. (7) suggests. The Lambert W function provides a more accurate scaling for the Gaussian limiting form found by Bleher using the \( \ln(\ln(t)) \) scaling (see the inset of Fig. 3). In addition, the Kummer function’s term in Eq. (5) yields for large \( r_j \), the power-law behavior \( P(r, t) \propto |r_j|^{-3} \). These non-Gaussian tails which decay with an exponent \(-3\) are clearly related to the fat tail of the flight times PDF \( \psi(\tau) \propto \tau^{-3} \). It follows that the Lambert scaling and Kummer correction found here are a required necessity for a numerical analysis, as seen in Fig. 3. Equation (5) represents the packet’s PDF very well, and as such one can disregard its correction \( \sim \mathcal{O}(1/\Omega^2(t)) \).

Our solution Eq. (5) contains three parameters, i.e., \( \langle \tau \rangle, \tau_0 \), and \( C_\psi \), all of which are able to be extracted out of our geometrical theory for the CDF of the flight times [Fig. 1(c)], as mentioned (see SM [27]). Furthermore, using our solution we are able to find a closed-form expression for \( \tau_0 \), given previous rigorous results for \( \langle \tau \rangle \); Considering extremely-long-time durations for Eqs. (5) and (6), namely, \( t \) for which \( \Omega(t) \simeq \ln(t) \), yields a Gaussian profile with a variance of \( \sigma^2 = \mathcal{O}(\ln(t)) \), where \( \sigma^2 = \mathcal{O}(2T) = \tau_0^2/2 \langle \tau \rangle \). In Ref. [19], it was rigorously proven that for \( t \to \infty \) the random variable \( \{r(t) - r(0)\}/\sqrt{\ln(t)} \) converges in distribution to a Gaussian variable with a zero mean and a variance \( \sigma^2 \) which is given by the scatterers’ radius as

\[
\sigma^2 = \frac{2(1 - 2R^2)}{\pi(1 - \pi R^2)},
\]

while for the mean time between collisions one has [18]

\[
\langle \tau \rangle = \frac{1 - \pi R^2}{2R}.
\]
Thus, using the above, we find for $r_0$,
\begin{equation}
    r_0 = \sqrt{2(\tau_0)^2} = \sqrt{2 \pi R (1 - 2R)},
\end{equation}
with an agreement to its leading behavior found in Ref. [21]. Comparing Eq. (10) with the values obtained via our geometrically calculated $\psi(\tau)$ gives a good agreement for radii in the range $(1/\sqrt{3}, 1/2)$. Hence, the only parameter which requires the computation of $\psi(\tau)$ is $C_\psi$, and the tail of $\psi(\tau)$ Eq. (1) is found in closed form.

Discussion and summary. In Ref. [18], an interesting doubling effect was pointed out. While for familiar diffusion processes, e.g., Brownian motion, the Gaussian packet’s variance is equal to the mean-square displacement (MSD), in this case there exists a factor of 2 between them. It arises from the fat-tail behavior of the packet of particles, as the MSD has two contributing elements, the far tail $\sim |r|^{-3}$ found here and the Gaussian salt. As half of the MSD can be explained using the Gaussian approximation, one needs to go beyond it. In this sense, the power-law tail is needed for a correct description of the MSD, which is the standard quantifier of diffusive processes. Calculation of the MSD demands the introduction of a far-tail cutoff, namely, the density is zero beyond $|r| = \tau$ (see Figs. 2 and 3). In order to receive a full description of the problem, one must construct a theory moving from that end point $|r| = \tau$ inward, e.g., to introduce the infinite covariant density $[31]$.

Our theory provides a description for the dynamics of the two-dimensional infinite-horizon LG based on the LW approach. With a correct choice of $F(\psi)$ and an appropriate calculation of $\psi(\tau)$, this theory can be extended to arbitrary lattice geometries, as well for other models and systems which exhibit similar features to the infinite-horizon LG model $[32–36]$. Importantly, since the power-law behavior Eq. (1) is valid for any spatial dimension $d < 6$ of the LG, so do our findings. While for the intermediate times we found smooth behavior of the particle’s PDF, for short enough times one finds oscillations in $P(r,t)$ (see Fig. 1 of Ref. [18]). These clearly originate from the staircase-like structure of $CDF(\tau)$ [see Fig. 1(c)].

Finally, we have carried out numerical simulations of a one-dimensional chain of stadium billiards [7]. We found that the PDF produced by this model perfectly fits a one-dimensional variant of Eq. (5). This is further evidence that our findings are universal and irrespective of the system’s spatial dimension, assuming the infinite-horizon and chaotic (renewal) conditions are met.

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