Finite-time Lyapunov exponent for a random Ehrenfest gas

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Abstract

We consider the motion of a system of free particles moving in a plane with hard scatterers of regular polygonal shape arranged in a random manner. Calling this the Ehrenfest gas which is known to be pseudo-integrable, we propose a finite-time Lyapunov exponent characterizing the dynamics. In the limit of large number of vertices, where polygon tends to a circle, we recover the Lyapunov exponent for the Lorentz gas. To obtain this result, we generalized the reflection law of a pencil of rays incident on a polygonal scatterer in a way that the formula for the circular scatterer is recovered in the limit of infinite vertices. Thus, seemingly paradoxically, chaos seems to emerge from pseudo-chaos.
1 Introduction

An understanding of the simultaneous occurrence of stochastic time evolution at a macroscopic level and deterministic evolution at a microscopic level poses one of the greatest challenges. Underlying equilibrium and transport properties of many-body systems is the chaotic microscopic motion - a hypothesis that was tested experimentally more than fifteen years ago [1]. Considering the Brownian movement of a colloidal particle in water, it was shown that the sum of positive Lyapunov exponents is positive. Since Lyapunov exponents measure whether the dynamics sensitively depends on the initial conditions, this quantity seemed to present for the first time a direct connection of microscopic dynamical instability to relaxation properties of a many-body system. The latter was propounded in the classic work of Krylov [2]. Krylov argued the case for mixing dynamics as a requirement for statistical laws to hold.

Subsequent to the work by Gaspard et al., there has been a vibrant debate where, mainly, at the centre of the debate is the Lorentz gas with polygonal scatterers. Due to the similarity with the model introduced by Ehrenfest, we call this model the Ehrenfest gas (Lorentz gas is the system with particles moving freely in a plane where circular scatterers are arranged in some manner). Due to the straight segments of the scatterers, there is no exponential separation of nearby trajectories and thus the Lyapunov exponent is zero for the Ehrenfest gas. However, (numerical) experimentally, it turns out the Brownian-like motion is exhibited by the Ehrenfest gas [3]. By Pesin’s theorem, the sum of positive Lyapunov exponents is equal to the Kolmogorov-Sinai entropy, $h_{KS}$ for closed systems [6]. For open systems, the difference between this sum and $h_{KS}$ gives the escape rate [7]. For systems like Ehrenfest gas, the analogues of Pesin theorem or Gaspard-Nicolis formula are not known. We believe that this important debate cannot be settled unless these analogues are found. Here we take a step in this direction by providing a definition of an exponent for such systems. This has been done by a suitable modification of the well-known Sinai formula [14] based on the change in curvature of incident pencil of rays upon reflection from a circular scatterer. It turns out that the adaptation constitutes a systematic generalization. We restrict ourselves to a regime of low density of scatterers, since the well-known results for Lorentz gases as well as our results and simulations break down in the opposite limit.

The dynamics of the polygonal billiard is described by the interval-exchange transformations [8,9]. These transformations are also employed to describe the act of “shuffling and cutting” of a pack of cards - which admittedly gives its clear visual description also. For mixing dynamical systems, it is well-known that stretching and folding is the fundamental operation, leading to the appearance of Smale horseshoe, and chaos follows. This, indeed, is also the case when we discuss mixing of fluids [10,11]. However, on
Figure 1: A pencil of rays incident on a disc of radius ‘a’ scatters such that the radius of curvature of the wavefront corresponding to them changes from $\rho_-$ to $\rho_+$. 

the other hand, granular flow is described by interval exchange transformations where an analogue of mixing can be achieved by shuffling and cutting \[13\]. Thus, in the case of Ehrenfest gas, we expect a Lyapunov exponent to be defined over a finite time, parallel to the connection between dynamical systems and continuum mechanics \[10\].

2 Collision rule

To motivate the definition of finite-time Lyapunov exponent for polygonal scatterers, we need to find the rule by which the radius of curvature changes upon a collision. In the case of circular scatterers (Lorentz gas), the change is given by the well-known reflection formula for spherical mirrors (Fig. 1):

$$\frac{1}{\rho_+} = \frac{1}{\rho_-} + \frac{2}{a \cos \varphi}.$$ (1)

Note that in the case of a Lorentz gas with low density $\rho_-$ is very large, and hence according to this equation $\rho_+$ is approximately $a/2$ or smaller.

In the case of polygonal scatterer, there is a similar scattering (Fig. 2). The formula, though, is different and requires a generalization of \[11\]. Referring to Fig. 3, the change in radius of curvature is given by

$$\rho' = \rho \left( \frac{\sin \alpha}{\sin(\alpha - 2\theta)} \right) \left( \frac{1 - \nu \cos \theta - \nu \sin \theta \tan \xi}{1 - \nu \cos \theta + \nu \sin \theta \tan \xi} \right).$$ (2)
Figure 2: A pencil of rays incident about a vertex of a polygonal scatterer, where the radius of curvature of the wavefront changes from $\rho_-$ to $\rho_+$. 

with $\nu = s_1/s_2$ and $\xi = (\alpha + \pi + 2\varphi - \theta)/2$.

The change in radius of curvature depends on where the pencil of rays strikes the scatterer. This is specified by the distances from the vertex, $s_1, s_2$. The perpendicular distance of the incident direction from the centre of a scatterer is $y$. Assuming a uniform distribution for $y$ and $\varphi$ (Fig. 3), we see that $s_1, s_2$ are also uniformly distributed. Denoting by $k$ the “diameter” (longest diagonal) of a scatterer, $s_1$ and $s_2$ can be derived using simple trigonometry in terms of $y, \varphi$:

$$s_1 = \frac{k \sin \varphi - y + \rho_- \sin(\alpha/2)}{\sin(\varphi + \theta/2)},$$

$$s_2 = \frac{-k \sin \varphi + y + \rho'_- \sin(\alpha/2)}{\sin(\varphi - \theta/2)},$$

$$\rho'_- \approx -\rho_- \cos(\theta - \alpha).$$ (3)

Moreover, the value of $\theta$ depends on whether the incident pencil of rays included an edge (which means two vertices) or a single vertex, and so on (see Fig. 4). The angle $\theta$ can be written in terms of the actual angle of the polygon, $\mathcal{T}$ and the number of vertices that lie between the two endpoints of the incident pencil of rays:

$$\theta = n_v \mathcal{T} - (n_v - 1)\pi.$$ (4)

To express $n_v$, we use a quantity $x$, which is the ratio of the distance between the two ends of the pencil, and, the projected length of one face of the
Figure 3: Geometry of reflection off a polygonal mirror. A pencil of rays with angular width $\alpha$ is incident such that its two ends strike two adjacent sides containing a vertex. The distance from the vertex of the points where the ends meet are $s_1$ and $s_2$. The perpendicular distance between the incident direction and the centre of the scatterer, $C$ is $y$. The change in radius of curvature upon such a reflection is given by Eq. 2.
Figure 4: (a) If the pencil of rays is incident about a vertex, $\theta = \pi - 2\pi/N$. (b) If it is incident such that it includes a side of the scatterer, then $\theta = \pi - 2 \times 2\pi/N$.

polygon:

$$x = \frac{\rho a \cos \phi}{a \cos \phi}.$$  \hspace{1cm} (5)

Thus,

$$n_v = \begin{cases} 
\text{Ceil}[x], & \text{with probability } \frac{\text{frac}[x]}{\text{floor}[x]}, \\
\text{Floor}[x], & \text{otherwise}; 
\end{cases}$$  \hspace{1cm} (6)

We have assumed that it is only the ratio, $x$, that is important for deciding the number of vertices. This is an approximation, since the projected lengths of all the sides is not the same. The value that we have used is only the largest projected length possible for all sides of the polygon. The actual projected side-length is not be constant for all sides, but we have made this assumption for the sake of simplicity. This number changes the effective value of $\theta$. However, we believe that this simplification does not affect our main results.

Substituting Eqs. (3, 4) in (2), we get a distribution for $\rho$ that peaks at the value obtained using the mirror formula. Moreover, as the number of vertices, $N$ increases the peak becomes sharper and sharper. In the limit of $N \to \infty$, as polygonal scatterer becomes circular, the distribution resembles the Dirac $\delta$ peaked at the value obtained using the mirror formula.

To show this, we plot the mode and variance of the distribution obtained for $\rho$ by the generalized reflection formula in Figs. 5 and 6 respectively. As
would be expected for any function approaching a Dirac $\delta$ function, the graphs show that the variance $\sigma \to 0$ as $N \to \infty$ and the mode $\mu$ goes to a fixed value, as obtained by (3). This establishes that (2) is a generalization of the (circular) mirror formula. This is an important result on which the subsequent discussion is based. It is appropriate to emphasize that the generalization is quite non-trivial.

3 Generalized Lyapunov exponent

We briefly discuss the estimation of Lyapunov exponent for the Lorentz gas, following Sinai [12, 14]. This motivates the approach of calculating an appropriate exponent for the Ehrenfest gas.

3.1 Circular scatterers

In the case of random Lorentz gas, it is well-known that the separation of the trajectories after $i^{th}$ collision, $s_i$ can be iteratively written as

$$s_i = s_{i-1} \left( \frac{\rho_i + v \tau_i}{\rho_i} \right)$$

(7)
Figure 6: We have plotted the variance of the distributions in the same cases as used in Fig. [5]. The expected trends have been described in the text. Note that this is also a log-linear plot.

where $\tau_i$ is the time of flight between the $(i-1)^{th}$ and the $i^{th}$ collisions. Given the initial separation $s_0$, after $n$ collisions and a long time, $T$,

$$s_n = s_0 \prod_{i=1}^{n} \left( \frac{\rho_i + v\tau_i}{\rho_i} \right)$$

$$= s_0 \exp \left[ T \sum_{i=1}^{n} T^{-1} \log \left( 1 + \frac{v\tau_i}{\rho_i} \right) \right]. \quad (8)$$

The Lyapunov exponent [14] is defined as the weight of the exponent in the separation of the trajectories of two close-by trajectories. From the above equation, the Lyapunov exponent can be identified as [14]

$$\lambda = \lim_{n,T \to \infty} \frac{1}{T} \sum_{i=1}^{n} \log \left( 1 + \frac{v\tau_i}{\rho_i} \right)$$

$$= \lim_{T \to \infty} \frac{v}{T} \int_{t_0}^{t_0 + T} \frac{1}{\rho(t)} dt. \quad (9)$$

For a dilute gas, $\rho$ is large compared to $a$; thus, just after a collision, we may write $\rho'$ as $(a \cos \phi)/2$ (even as $a/2$). This is the analogy of the image of a far-away object in a convex mirror. Denoting the mean free path and mean free time by $\mu_f$ and $\tau_f$ ($= \mu_f/v$) respectively, we can approximate the long time $T$ by $N\tau_f$. Thus the Krylov estimate [2] for the Lyapunov exponent can be obtained by realizing that the mean free path goes as the inverse of
the number density of the scatterers, \( n_s \):

\[
\lambda \sim \frac{1}{\tau_f} \left\langle \log \left( 1 + \frac{2\mu f}{a} \right) \right\rangle \\
\sim n_s \log \frac{1}{n_s}.
\]  

(10)

In fact, realizing that \( \{v\tau_i\} \) are distributed according to an exponential distribution with a weight of the mean free path, and performing the average with this distribution gives us a more correct formula,

\[
\lambda \sim n_s e^{n_s \Gamma(0, n_s)}
\]

(11)

where \( \Gamma(0, n_s) \) is the incomplete Gamma function. For low densities, this result is close to the formula derived by van Beijeren and Dorfman [15]:

\[
n_s (-\log n_s - C + 1)
\]

where \( C \) is the Euler-Mascheroni constant.

### 3.2 Polygonal scatterers

The Ehrenfest Gas can be contrasted with the Lorentz Gas by the way in which the angles between two nearby rays change upon reflection. In the case of the Lorentz Gas, the initial angle \( \alpha \) can be made arbitrarily small. Since the new angle \( \alpha' \) is given by

\[
\alpha' = \alpha \left( \frac{\rho}{\rho'} \right).
\]  

(12)
\( \alpha \) can be chosen to make \( \alpha' \) as small as necessary. In the Erhenfest Gas, the expression for change in angle is

\[
\alpha' = 2\pi - 2\theta + \alpha.
\]

(13)

This expression is additive in nature. If the ray hits a vertex, \( \theta < \pi \) and even by choosing \( \alpha \) to be arbitrarily small, \( \alpha' \) cannot be made as small as necessary.

In a low density Lorentz gas, \( \rho \) increases uniformly with time until it falls to about \((a/2)\) after a collision, and subsequently continues to increase uniformly. The pattern continues as long as both of the nearby rays hit the same scatterer. This condition enforces an upper bound on \( \rho \alpha' \), and hence on \( \alpha' \) and \( \alpha \). By choosing the initial angle \( \alpha \) to be arbitrarily small, this condition can be satisfied for all times.

For polygonal scatters, since \( \alpha' \) cannot be made arbitrarily small, the rays do not hit the same scatter after a finite number of collisions. Also, when the pencil of rays falls on a flat side, the radius of curvature continues to increase uniformly and falls only when the rays hit a vertex.

In the \( \rho - t \) schematic graph shown in Fig. 8 for a Lorentz gas the sawtooth nature of the graph continues indefinitely, since as discussed above, the rays can always be made to hit the same scatterer. However, for the Erhenfest gas, the condition is necessarily violated after a finite number of collisions and the graph terminates. This termination is representative of the fact that beyond this time the two rays hit different scatterers, and continue in entirely uncorrelated trajectories, without a well defined radius of curvature. This is the fundamental reason for the existence of a finite-time Lyapunov exponent in such systems.

Also, in these plots, we have assumed that the distance between any two scatterers is equal to the mean free path, and hence the height of all teeth in the first graph is the same. However, in the second case, for the polygonal scatterer, at each collision the value of \( \rho \) may not fall, since the two nearby rays can hit a flat side of the polygon, effectively causing no change to the value of \( \rho \).

In analogy to the circular scatterers, for the polygonal scatterers we define the finite-time Lyapunov exponent as

\[
\lambda_f = \frac{N}{T} \sum_{i=1}^{N} \ln \left( 1 + \frac{2\tau_i u}{\alpha} \right).
\]

(14)

The above expression is the same as the usual expression for the Lyapunov exponent, the only difference is that instead of averaging over a time \( T \) which goes to infinity, we average over a finite time. So, the average of the separation after that point would yield zero. A simulation was performed on Mathematica using the reflection formulae [2], giving estimates of \( N \approx 4 \) and \( T \approx 100 \) for an Ehrenfest Gas with a mean free path of 0.125 in units.
Figure 8: The $\rho - t$ graph for the Lorentz gas and Ehrenfest gas respectively. Note that this is only a schematic plot.

of the size of the scatterers. Scatterers with $10^5$ sides were chosen, with an initial angle between nearby rays taken to be around $3 \times 10^{-5}$ radians.

Since the Lyapunov exponent is $\langle \rho(t) \rangle$, it is clear from the $\rho - t$ graph shown that an infinite time-average makes sense only for the Lorentz system as the graph continues for an infinite time and thus would lead to a finite value for the Lyapunov exponent. For the Ehrenfest system, the (usual) Lyapunov exponent is always zero because an infinite time average of a quantity that is zero after a finite time, would obviously yield zero.

To evaluate the expression for $\lambda_f$, we need a distribution function that takes into account the different lengths of the “teeth” in the $\rho - t$ graph for the Ehrenfest system. Writing this distribution function involves determination of the number of collisions that two rays undergo on a straight edge before eventually encountering a vertex. We calculate the probability that the two rays encounter a vertex in the $k^{th}$ collision with a scatterer. We assume that the distance between any two scatterers is equal to the mean free path $\mu_f$ between the scatterers. Let the probability of hitting a vertex in the first collision be $p$. This is proportional to $\rho \alpha = \mu_f \alpha$ which is the distance between the two end points of the rays. If it misses (with a probability of $(1 - p)$), it has hit a flat surface, and the separation of the rays just before it hits the next scatterer is proportional to $2\mu_f \alpha$, and the probability of hitting a vertex then is $2p$. The probability for it to miss the second one is $(1 - 2p)$. The ray hits the $k^{th}$ vertex only if it misses the vertex on the
first \( k - 1 \) collisions with a probability of \((1 - p)(1 - 2p)...(1 - (k - 1)p)\) and hits the \( k^{th} \) vertex with a probability \( kp \). Combining these, the distribution function is written as

\[
f(k, p) = (1 - p)(1 - 2p)...(1 - (k - 1)p)kp.
\]

Once \( kp > 1 \), the two rays definitely hit across a vertex, and for larger \( k \) the probability \( f(k, p) \) must be zero. The condition of \( kp > 1 \) is equivalent to \( k > \text{Ceil}[1/p] \), since \( k \) is an integer. Thus the support of this distribution is the set of integers from \( \{1, ..., \text{Ceil}[1/p]\} \).

For the purposes of simplicity we have assumed that \( p \) is independent of \( \phi \). We assume that the probability \( p \) is approximately as if the rays were striking the polygon with \( \phi = 0 \), and we approximate \( p = \frac{\mu/\rho}{2a\sin(\pi/N)} \). However, the probability \( p \) in itself changes at every collision with a vertex. For the next value, \( p \) would be proportional to the value of \( \alpha \) after collision, i.e. \( \alpha' \). This gives a new probability \( p' \). We can relate \( p \) and \( p' \) using the relations between \( \alpha \) and \( \alpha' \) (Eq. 13). This has been discussed below in further detail.

We now derive a formula to calculate the finite-time Lyapunov exponent for this Ehrenfest system. In Eq. (14) \( \tau_i \) follows a distribution governed by \( f(k, p) \) defined earlier. The new \( \tau_i \) is \( i \times \tau_f \), where \( i \) is taken from the distribution \( f(i, p) \) (same as \( f(k, p) \) as defined earlier). Correspondingly, the time over which we average out is also \( i \times \tau_f \). Thus, the averaging over the distribution \( f \) gives us the finite-time Lyapunov exponent for a single tooth:

\[
\lambda_f = \frac{1}{\tau_f} \sum_{i=1}^{\text{Ceil}[1/p]} \frac{1}{i} \ln \left(1 + \frac{2i \times \tau_f v}{a}\right) f(i, p).
\]

The crucial point here is that \( f(i, p) \) in itself is more than just a simple function of \( i \). It also depends on the probability \( p \) of the two ends of the pencil of rays hitting across a vertex (or vertices). If we wish to average over multiple teeth we have to add a summation and an index, \( j \), running over the teeth. The probability \( p \) is now be represented by \( p_j \), since it changes at every step. This results in an expression of the form

\[
\lambda_f = \frac{1}{\Lambda \tau_f} \sum_{j=0}^{\Lambda-1} \sum_{i=1}^{\text{Ceil}[1/p_j]} \frac{1}{i} \ln \left(1 + \frac{2i \times \tau_f v}{a}\right) f(i, p_j)
\]

where we have averaged over \( \Lambda \) teeth. Here, \( p_j \) is a probability which is proportional to \( \alpha \) at that tooth, and increases with \( j \). An explicit equation for \( p_j \) can be calculated using the relations between \( \alpha' \) and \( \alpha \) to give:

\[
p_j = p_{j-1} + \frac{(2\pi - 2\theta) \rho}{2a \sin(\pi/N)}.
\]
Figure 9: The solid curve corresponds to the Lyapunov exponent for the Lorentz gas and the dashed curve corresponds to that for the Ehrenfest gas, both plotted as a function of the scatterer density. The left panel corresponds to an initial $p = 0.01$ and the right panel corresponds to $p = 0.9$.

Note however that $\theta$ itself is not a constant, and varies for each tooth. Thus determining an analytical expression for the average over multiple teeth is not an easy task. We present the analytic results for the Lyapunov exponent as calculated for the first tooth in Fig. 9. We plot the results for various $p$ and compare those with the result for the Lorentz gas. Note that the value of $p$ for the initial collision is effectively a measure of $N$, and as the initial $p \to 1$, $N \to \infty$. As $p \to 1$, it can be seen that the results for the Ehrenfest gas approach those for the Lorentz gas.

However, we claim that the Lyapunov exponent, calculated over a single tooth, gives a lower bound on the more accurate Lyapunov exponent that is calculated by performing an average over multiple teeth. We now present a heuristic argument supporting this claim. Note that in general, there are two trends in the sizes of the teeth. The first few teeth follow a ‘dynamic’ trend, wherein the size of the teeth in general decreases with tooth number. This is because after every tooth the value of $\alpha$ increases, and the rays encounter a vertex with a greater probability. Subsequently, the tooth is shorter. This general decreasing trend is expected until $\text{Ceil}[1/p]$ becomes 1. After this point, we enter the ‘static’ trend, wherein the rays have diverged sufficiently for them to hit across a vertex at every collision with a scatterer. Thus all teeth beyond this point exist only for the time the rays have travel between any two scatterers, a time which we have approximated to be $\tau_f$. This can also be seen by noting that $\text{Ceil}[1/p]$, remains fixed at 1 for all $p$ beyond a certain value. Thus, the teeth in this region are of the same ‘size’.

The general equation for a Lyapunov exponent gives us $\lambda = \frac{\ln(\rho_t)}{t_1 - t_0}$. If we only look at a single tooth, then the value of $\rho(t)$ increases linearly with time. Thus, in the expression for $\lambda$, the numerator increases at a logarithmically, but the denominator increases linearly. This would imply, that for a smaller tooth, $\lambda$ is larger, and vice versa. If we average over multiple teeth rather than just the first tooth, we include averages over teeth which contribute to larger values of $\lambda$, and the overall Lyapunov exponent as calculated over the
first tooth shall be a lower bound on the Lyapunov exponent as calculated by an average over multiple teeth.

The picture suggested above has been verified via a simulation on Mathematica as well. In Fig. 10 we have shown that not only are the simulation results for a single tooth agreeing well with the estimate of the finite-time Lyapunov exponent as calculated with an average over a single tooth, but also clearly the finite-time Lyapunov exponent as obtained by averaging over multiple teeth is greater than what is obtained for a single tooth.

4 Summary

The relation of microscopic dynamics and diffusion or general transport properties is of a great fundamental importance. Last twenty years have witnessed a rather interesting discussion, beginning from the work by Gaspard at al. [1]. The contentious case - called here as the Ehrenfest gas - consists of point particles subjected to scattering from fixed polygonal-shaped hard scatterers. In this work, we have proposed a systematic treatment of this problem. The reflection law for the case of a regular polygonal scatterer is given here. We have not found this result in literature, quite surprisingly. This result is crucial for any further progress. Having found this, we have
argued that for pseudo-integrable systems (which are non-chaotic), it is natural to define a finite-time Lyapunov exponent. The exponent found here is of particular significance because in the limit of the number of vertices becoming infinite (and hence the scatterer becoming circular), the exponent for the Lorentz gas is recovered. Thus, on both counts - the collision rule and Lyapunov exponent - we have generalized the results; thence, it is demonstrated that the Lorentz gas is a special case of the Ehrenfest gas. These results pave the way for an understanding of the connection of “diffusion” and pseudo-integrable dynamics. It is clear from the results given here that diffusion of certain kind will certainly be possible in the presence of “pseudo-chaos”. We believe that, in a way similar to the finite-time Lyapunov exponent defined here, there would be suitable generalizations of Pesin’s theorem and Gaspard-Nicolis formula for the Ehrenfest gas.

These results are essential for developing an understanding of the relationship of microscopic dynamics and transport properties like diffusion. We believe that the formulae found here apply not only to the pseudo-integrable Hamiltonian flows but also to granular flows where the dynamics is more akin “shuffling and cutting” rather than “stretching and folding”.

Acknowledgements

S.M. and S.C. would like to thank the National Initiative for Undergraduate Sciences (NIUS) program under the Homi Bhabha Centre for Science Education (HBCSE), Mumbai for the opportunity and funding for this work.
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