

Lyapunov Exponents and Anomalous Diffusion of a Lorentz Gas with Infinite Horizon Using Approximate Zeta Functions

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We compute the Lyapunov exponent, the generalized Lyapunov exponents, and the diffusion constant for a Lorentz gas on a square lattice, thus having infinite horizon. Approximate zeta functions, written in terms of probabilities rather than periodic orbits, are used in order to avoid the convergence problems of cycle expansions. The emphasis is on the relation between the analytic structure of the zeta function, where a branch cut plays an important role, and the asymptotic dynamics of the system. The Lyapunov exponent for the corresponding map agrees with the conjectured limit $\lambda_{\text{map}} = -2 \log(R) + C + O(R)$ and we derive an approximate value for the constant C in good agreement with numerical simulations. We also find a diverging diffusion constant $D(t) \sim \log t$ and a phase transition for the generalized Lyapunov exponents.

KEY WORDS: Lyapunov exponents; anomalous diffusion; Lorentz gas; zeta functions; branch points.

1. INTRODUCTION

Perhaps the best-known measure of a chaotic system is the Lyapunov exponent. In the theory of chaotic dynamics one is of course interested in calculating this and similar quantities, either by finding analytical estimates or by devising effective calculation schemes,⁽⁵⁾ but often one finds oneself compelled to use numerical simulation. This is unsatisfactory since it is not an easy task to extract information on the asymptotic behavior from numerical data.

Various averages of chaotic systems are obtainable via transfer operators and their Fredholm determinants or *zeta functions*. This is a beautiful formalism, but the best results are obtained for a very restricted class of chaotic systems, namely those fulfilling Axiom A. This is because Axiom A guarantees nice analytical features of the zeta functions⁽¹⁻⁴⁾

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yielding rapidly, convergent cycle expansions enabling efficient deduction of its leading zeros.⁽⁵⁾ Applications of cycle expansions to non-Axiom A systems are not very successful.^(6, 7)

In this paper we will study a system which is far from the textbook 1d Axiom A map, namely the two-dimensional Lorentz gas on a square lattice. This is a Hamiltonian system with two degrees of freedom, continuous time, and infinite symbolic dynamics. We will demonstrate that zeta functions may be of use even here. The key point is that we will avoid writing the zeta function in terms of periodic orbits, as that would lead to divergence problems that we could not handle. The price we will pay is that our zeta functions are no longer exact, but they are approximate in a sense that does not affect the leading zero very much. The averages we will compute are directly related to the motion of this leading zero with respect to variations of a parameter. However, matters will be complicated if there are nonanalyticities in the vicinity of the leading zero, like branch cuts. This is, we believe, a generic feature of intermittent systems. Such singularities will cause problems for cycle expansions but do carry important information about the asymptotic dynamics. In the Lorentz gas there will be a branch cut reflecting the existence of the infinite horizon. It will not prevent the Lyapunov exponent from being well defined, but will yield a diverging diffusion constant. It will also imply a phase transition for the generalized Lyapunov exponents.

The purpose of the present paper is to focus on the main principles of how chaotic averages may be computed from zeta functions exhibiting singularities close to the leading zero. In the calculation of Lyapunov exponents we will therefore be satisfied with a rather crude approximation of the zeta function, but still derive expressions in good agreement with numerical data in the small-scatterer limit. In the computation of diffusion the necessary details of the zeta function may be refined considerably with relative ease and we will arrive at what appears to be the exact result.⁽¹³⁾

In Section 2 we review the necessary theory. In Section 3 we perform all calculations and we then end with some comments in Section 4.

2. THEORY

2.1. Lyapunov Exponents and Zeta Functions

The largest Lyapunov exponent is defined by

$$\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \log |A(x_0, t)| \quad (1)$$

provided the limit exists and is independent of the initial point x_0 (except for a set of measure zero). $A(x_0, t)$ is the largest eigenvalue of the Jacobian along the trajectory starting at x_0 and evolving during time t .

If $A(x_0, t)$ is multiplicative along the flow, as it is for one-dimensional systems, one can use ergodicity and write it as a phase space average

$$\lambda = \frac{1}{t} \int \rho(x) dx \log |A(x_0, t)| \equiv \frac{1}{t} \langle \log |A(x_0, t)| \rangle \quad (2)$$

where $\rho(x)$ is the invariant density and t is arbitrary. If $A(x_0, t)$ is not multiplicative along the flow (as is the case for systems with more than one dimension), one has to take the $t \rightarrow \infty$ limit in (2). Whether or not we take the $t \rightarrow \infty$ limit, it will reappear when we expand the invariant density in terms of periodic orbits (see below and Appendix).

We now want to formulate the Lyapunov exponent in terms of zeta functions, but first we demonstrate how the average of an observable may be expanded in terms of periodic orbits. We associate the observable $w(x_0, t)$ with the trajectory starting at x_0 and evolving during time t . This evolution is described by the function $x = f^t(x_0)$ (saying that the initial point x_0 is mapped onto x during time t). Moreover, we assume that the observable w is multiplicative along the flow, that is,

$$w(x_0, t_1 + t_2) = w(x_0, t_1) w(f^{t_1}(x_0), t_2)$$

The average of w may be written as the following periodic orbit sum (see Appendix):

$$\lim_{t \rightarrow \infty} \langle w \rangle = \lim_{t \rightarrow \infty} \sum_p T_p \sum_{n=1}^{\infty} w_p^n \frac{\delta(t - nT_p)}{|\det(1 - M_p^n)|} \quad (3)$$

where n is the number of repetitions of primitive orbit p having period T_p , and M_p is the Jacobian (transverse to the flow). w_p is the weight associated with cycle p . This expression can be given a compact representation in terms of the evolution operator \mathcal{L}'_w . This operator is defined by its action on a phase space density $\Phi(x)$,

$$\mathcal{L}'_w \Phi(x) = \int w(y, t) \delta(x - f^t(y)) \Phi(y) dy \quad (4)$$

The average (3) can formally be written as the trace of the weighted evolution operator (cf. Appendix)

$$\lim_{t \rightarrow \infty} \langle w \rangle = \lim_{t \rightarrow \infty} \text{tr} \mathcal{L}'_w \equiv \lim_{t \rightarrow \infty} \int w(x, t) \delta(x - f^t(x)) dx \quad (5)$$

We do not address the question of whether the trace may be interpreted as a sum over eigenvalues.

Zeta functions are introduced by observing that the trace may be written as

$$\text{tr } \mathcal{L}'_w = \frac{1}{2\pi i} \int_{-\infty - ia}^{\infty - ia} e^{ikt} \frac{Z'_w(k)}{Z_w(k)} dk \tag{6}$$

For a Hamiltonian system with two degrees of freedom the zeta function reads⁽⁸⁾

$$Z_w(k) \prod_p \prod_{m=0}^{\infty} \left(1 - w_p \frac{e^{-ikT_p}}{|A_p| A_p^m} \right)^{m+1} \tag{7}$$

where A_p is the expanding eigenvalue of M_p .

The equality between Eqs. (3) and (6) can readily be verified by the reader. We only want to stress two points. (a) To be mathematically unambiguous the delta functions should be understood as, e.g. Gaussians and the Fourier transform (6) performed over the corresponding Gaussian window.⁽⁹⁾ When going from (6) to (3) it is essential that the infinite product (7) converge so that summation and integration may be interchanged. This is the case if the constant a in (6) is sufficiently large so that the contour goes below the leading zero of (7).

Cycle expansions of the zeta functions generally have better convergence properties than the infinite product representation (7) since they converge beyond the leading zero and up to the first singularity.⁽⁵⁾ The zeta function is entire for Axiom A systems,⁽⁴⁾ which makes cycle expansions very successful for this special case. In this paper we will consider cases where the zero is also a singularity (branch point), so a cycle expansion will not converge even there and the zeta function is rather useless as it stands. We return to these problems in Section 2.3.

We must now find a weight w appropriate for computing the Lyapunov exponent. The quantity whose average we are going to study is $\log |A(x_0, t)|$, which is certainly not multiplicative. In fine dimension we can study the average of the multiplicative weight $w = |A(x_0, t)|^{\tau}$ and obtain the Lyapunov exponent by differentiation

$$\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \left. \frac{d \text{tr } \mathcal{L}'_{\tau}}{d\tau} \right|_{\tau=0} \tag{8}$$

In two-dimensional systems, such as the Lorentz gas, the weight is multiplicative only along the periodic orbits. But this is exactly where we evaluate our weights, so this departure from exact multiplicativeness does

not affect the validity of our considerations and all our expression are valid for this case as well. In ref. 10 the authors modify the weighted evolution operator to achieve the desired semigroup property. The modifications affect the analytic structure of the zeta functions high up in the complex k plane and have no implications for our results.

The leading zero $k_0(\tau) = -i \cdot h(\tau)$ is always on the negative imaginary axis if $\tau > 0$. For unitary reasons one has $k_0(0) = 0$. The leading zero provides the leading asymptotic behavior of the trace provided that there is a gap until next zero or singularity. In that case one would have

$$\lambda = \frac{d}{d\tau} h(\tau)|_{\tau=0} \quad (9)$$

We cannot take for granted that this expression is always valid.

Generalized Lyapunov exponents⁽¹¹⁾ $\lambda(\tau)$ are defined by considering the scaling behavior of $\langle |A(x_0, t)|^\tau \rangle$. If the leading zero is isolated, then $\langle |A(x_0, t)|^\tau \rangle$ will grow exponentially with t :

$$\lim_{t \rightarrow \infty} \langle |A(x_0, t)|^\tau \rangle = \lim_{t \rightarrow \infty} \text{tr } \mathcal{L}_\tau^t = \lim_{t \rightarrow \infty} e^{\lambda(\tau) \tau t} \quad (10)$$

so that

$$\lambda(\tau) = \frac{h(\tau)}{\tau} \quad (11)$$

The ordinary Lyapunov exponent is recognized as the limit $\lambda = \lim_{\tau \rightarrow 0} \lambda(\tau)$.

2.2. Diffusion Coefficients and Zeta Functions

We will consider the Lorentz gas obtained by unfolding the Sinai billiard. The coordinate in the unfolded system is called \hat{x} . The corresponding vector in the billiard (or the *unit cell*) is x . They are related by translation $\hat{x} - x \in T$, where T is the group of translations building up the Lorentz gas from the unit cell.

The diffusive properties can be extracted from the average

$$\langle e^{\beta \cdot (\hat{f}^t(x_0) - x_0)} \rangle_{x_0} \quad (12)$$

The average is taken over one unit cell. Again we must perform the trick of introducing a multiplicative weight and then by differentiation extract the average in which we are interested.

It was demonstrated in ref. 12 that this average can be computed by considering the dynamics in the unit cell only. This is obtained by inserting the weight

$$w(x, t) = e^{\beta \cdot (\hat{f}^t(x) - x)} \tag{13}$$

into the evolution operator (4). The diffusion constant is now given by

$$D = \lim_{t \rightarrow \infty} \frac{1}{\nu t} \sum_{i=1}^{\nu} \langle (\hat{f}^t(x_0) - x_0)^2 \rangle_{x_0} = \lim_{t \rightarrow \infty} \frac{1}{\nu t} \sum_{i=1}^{\nu} \frac{\partial^2}{\partial \beta_i^2} \text{tr } \mathcal{L}_\beta^t |_{\beta_i=0} \tag{14}$$

where the sum is taken over spatial components of the 2ν -dimensional phase space. (We conform with ref. 12 in the definition of D ; in some work, e.g., ref. 13, this differs by a factor of 2.)

So far all our expression, have been exact [although (5) lacks a rigorous proof]. We now turn to more approximate considerations.

2.3. Approximate Zeta Functions

In recent publications we have investigated a way of approximating zeta functions for intermittent systems.^(7, 9, 14) We call this the BER approximation after the authors of ref. 16. In an intermittent system laminar intervals are interrupted by chaotic outbursts. Let Δ_i be the time elapsed between two successive entries into the laminar phase. The index i labels the i th interval. Provided the chaotic phase is *chaotic enough*, the lengths of the intervals Δ_i are presumed uncorrelated, and Δ may be considered as a stochastic variable with probability distribution $p(\Delta)$. The zeta functions (unit weight $w = 1$) may then be expressed in terms of the Fourier transform of $p(\Delta)$

$$Z(k) \approx \hat{Z}(k) \equiv 1 - \int_0^\infty e^{-ik\Delta} p(\Delta) d\Delta \tag{15}$$

We refer to ref. 7 for a derivation. Due to the normalization of $p(\Delta)$ we see that leading zero $k_0 = 0$ is by construction exact because of probability conservation.

In order to compute the probability distribution we introduce a surface of section (SOS). This should, according to the BER prescription, be located on the border between the laminar and chaotic phases. We call the phase space of the SOS Ω and its coordinates x_s . The flight time to the next intersection is then a function of x_s : $\Delta_s(x_s)$. The probability distribution then reads

$$p(\Delta) = \int_{\Omega} \delta(\Delta - \Delta_s(x_s)) \rho_s(x_s) dx_s \tag{16}$$

where $\rho_s(x_s)$ is the invariant density, which is uniform, $\rho_s(x_s) dx_s = dx_s / \int_{\Omega} dx_s$, for a Hamiltonian ergodic system, assuming of course that the SOS coordinates are canonically conjugate.

It is straightforward to include weights in this formalism,⁽⁹⁾ such as the weight $w = |A(x_0, t)|^\tau$ introduced in Section 2.1. The local expansion factor over one interval $A_s(x_s)$ is also a function of x_s . The zeta function is then related to a generalized distribution

$$p_\tau(\Delta) = \int_{\Omega} |A_s(x_s)|^\tau \delta(\Delta - A_s(x_s)) dx_s \tag{17}$$

The zeta function $\hat{Z}_\tau(k)$ is obtained as

$$\hat{Z}_\tau(k) \equiv 1 - \int_0^\infty e^{-ik\Delta} p_\tau(\Delta) d\Delta \tag{18}$$

3. APPLICATION TO THE LORENTZ GAS

We now begin our study of the Lorentz gas on a square lattice. The lattice spacing is unity, each disk is circular with radius $R < 1/2$, and the point particle bouncing around has unit velocity. The unit cell of this system, the Sinai billiard,⁽¹⁷⁾ whose dynamics we will study, is indeed an intermittent system; there exist periodic orbits with arbitrarily small Lyapunov exponents $\log A_p/T_p$. The disk will define our SOS. We use the two angles ϕ and α defined in Fig. 1a as coordinates. The normalized measure is then $dx_s = d\phi d(\sin \alpha)/4\pi$. Consider now a segment of the trajectory between two disk collisions. This segment can be labeled according to the disk that would be hit in the unfolded system; the label $\mathbf{q} = (n_x, n_y)$ is the associated lattice vector.⁽⁹⁾ It is easy to realize that only disks associated with a coprime lattice vector may occur. We then partition the SOS into subsets $\Omega_{\mathbf{q}}$ where $\Omega_{\mathbf{q}}$ is the part of Ω for which the trajectory hits disk \mathbf{q} .

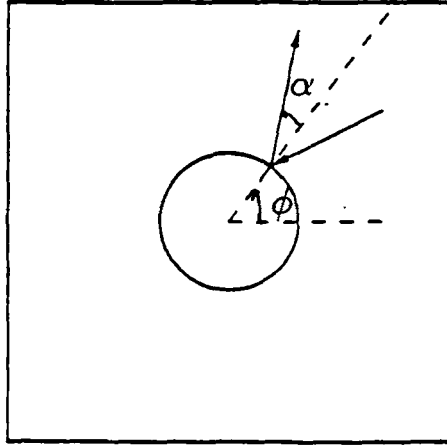
The purpose is now to apply the BER approximation to this system and compute Lyapunov exponents and diffusion constants.^(9, 14)

3.1. Calculation of $p_\tau(\Delta)$

We will illustrate our method by the following rather crude approximation of $p_\tau(\Delta)$ (the nature of the crudeness will be discussed below):

$$p_\tau(\Delta) \approx \begin{cases} \frac{4}{3} \frac{\Gamma((2-\tau)/2)^2}{\Gamma(2-\tau)} R^{1-\tau} \Delta^\tau, & \Delta \leq \frac{1}{2R} \\ \frac{4}{3} \frac{\Gamma((2-\tau)/2)^2}{\Gamma(2-\tau)} \frac{2^{\tau/2-3} R^{-\tau/2-2}}{\Delta^{3-3\tau/2}}, & \Delta > \frac{1}{2R} \end{cases} \tag{19}$$

a)



b)

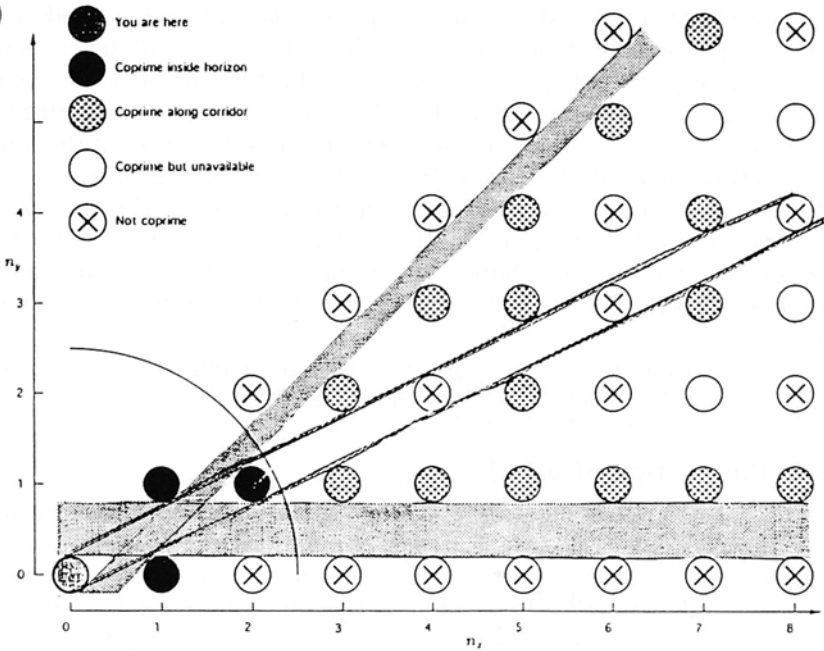


Fig. 1. (a) The Sinai billiard with definitions of the variables ϕ and α . (b) The unfolded system with free directions (corridors) indicated. (c) The region of integration in Eq. (27).

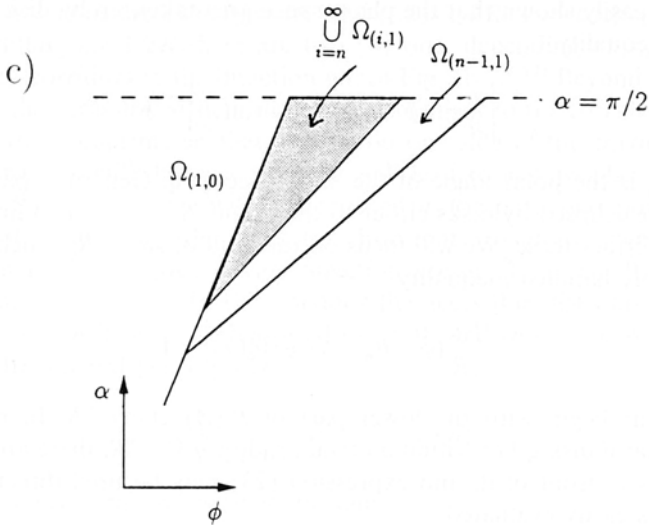


Fig. 1. (Continued)

This expression was used already in ref. 14, but as it plays a central role in this paper we present its derivation in some detail. Complementary details may be found in refs. 9 and 14.

We start from expression (17) for $p_\tau(\Delta)$. First we smear the distribution, that is, we replace the delta function with some extended distribution δ_σ . The exact form of this function is irrelevant; the only thing we assume is that it is wide: $\sigma \gg 1$. In most applications in this paper we are interested in evaluating the zeta function in the vicinity of $k = 0$ and it is evident that the smearing of $p_\tau(\Delta)$ will only have a minor effect there.

We now have

$$p_\tau(\Delta) = \sum_{\mathbf{q}} \int_{\Omega_{\mathbf{q}}} |A_s(x_s)|^\tau \delta_\sigma(\Delta - \Delta_s(x_s)) dx_s \tag{20}$$

The large width σ allows us to move the smeared delta function to the left of the integral sign because the variation of $\Delta_s(x_s)$ over $\Omega_{\mathbf{q}}$ is of the order $\sim R$ and we have $\sigma \gg 1 > R$. We have

$$p_\tau(\Delta) = \sum_{\mathbf{q}} \delta_\sigma(\Delta - q) \int_{\Omega_{\mathbf{q}}} |A_s(x_s)|^\tau dx_s \equiv \sum_{\mathbf{q}} \delta_\sigma(\Delta - q) a_{\mathbf{q}}(\tau) \tag{21}$$

We have chosen the length of the lattice vector $|\mathbf{q}| \equiv q$ as the average of $\Delta_s(x_s)$ over $\Omega_{\mathbf{q}}$. The local expansion factor is $|A_s(x_s)| = 2\Delta_s(x_s)/R \cos(\alpha)$ to leading order in R .

It is easily shown that the phase space area taken up by disk \mathbf{q} is given by the inequality

$$\left| \frac{q}{R} \sin(\phi - \theta_{\mathbf{q}} - \alpha) + \sin(\alpha) \right| < 1 \tag{22}$$

where $\theta_{\mathbf{q}}$ is the polar angle of the lattice vector \mathbf{q} . Generally parts of this region are eclipsed by disks closer to the origin. So in order to find $\Omega_{\mathbf{q}}$ one has to subtract these. We will focus on the limit of small R , which gives the more easily handled inequality

$$\left| \frac{q}{R} (\phi - \theta_{\mathbf{q}} - \alpha) + \sin(\alpha) \right| < 1 \tag{23}$$

Let us begin with the lower part of $P_{\tau}(\Delta)$: $\Delta < 1/2R$. In ref. 9 it is shown that if disk \mathbf{q} lies within a certain radius $q < 1/2R$, there are no eclipsing disks in front of it, and expression (23) may be used directly, so the integral is easily evaluated:

$$\begin{aligned} a_{\mathbf{q}}(\tau) &= \left(\frac{2q}{R}\right)^{\tau} \frac{1}{4\pi} \int_{\Omega_{\mathbf{q}}} \cos^{1-\tau}(\alpha) \, d\alpha \, d\phi \\ &\approx \frac{1}{\pi} \frac{\Gamma((2-\tau)/2)^2}{\Gamma(2-\tau)} \left(\frac{R}{q}\right)^{1-\tau} \end{aligned} \tag{24}$$

At this point we can make a simple consistency check on Eq. 24 by putting $\tau = 1$; this amounts to studying the topological zeta function. Then $a_{\mathbf{q}}(1) = 1$ and the trace is, as it should, just counting periodic orbits; see ref. 9 for more details.

In order to find an approximate expression for $p_{\tau}(\Delta)$ we must know the density of coprime lattice points, i.e., the average number $d_c(r) \, dr$ of such points having a distance between r and $r + dr$ from the origin [as this is a highly irregular function, one rather calculates its integral $\int_0^r d_c(r') \, dr'$]. One may then just copy the derivation of the summatory function of Euler's function $\Phi(t) = \sum_{n=1}^t \phi(n)$ with minor modifications.⁽¹⁸⁾ The leading-order result is $d_c(r) \sim (12/\pi) r$. (In ref. 14 we estimated d_c in a simple way, avoiding all number-theoretic intricacies; the result was only 2% wrong). This yields

$$p_{\tau}(\Delta) = \sum_{\mathbf{q}} \delta_{\sigma}(\Delta - q) a_{\mathbf{q}}(\tau) = \frac{12}{\pi^2} \frac{\Gamma((2-\tau)/2)^2}{\Gamma(2-\tau)} R^{1-\tau} \Delta^{\tau} \tag{25}$$

It is obvious that these considerations require many disks inside the horizon $1/2R$ to be justified. The results therefore apply in the limit of small R .

Next we consider the opposite limit, $\Delta \gg 1/2R$. For each (coprime) disk \mathbf{q} fulfilling $q < 1/2R$ there are two (or one, depending on symmetry) transparent corridors in the direction \mathbf{q} (see Fig. 1b).^(9, 13) Beyond this critical radius the accessible disks will be those adjacent to the corridors. (They still have to be coprime so they will lie on one side of the corridor only; see Fig. 1b). We will discover that this will lead to a power-law decay of $p(\Delta)$. For the moment, we will be interested in the particular power (as a function of τ) and not the prefactor. For that reason we perform our calculation in the corridor having direction vector $(1, 0)$, as all corridors provide the same power. In this corridor the accessible disks are the ones labeled $(n, 1)$. Disk $(n, 1)$ is shadowed by $(1, 0)$ and $(n-1, 1)$. We need to evaluate the integral [cf. Eq. (24)]

$$j_n \equiv \int_{\Omega_{\mathbf{q}=(n,1)}} \cos^{1-\tau}(\alpha) d\alpha d\phi \quad (26)$$

It is more convenient to consider the sum

$$J_n \equiv \sum_{i=n}^{\infty} j_i = \int_{\cup_{i=n}^{\infty} \Omega_{\mathbf{q}=(i,1)}} \cos^{1-\tau}(\alpha) d\alpha d\phi \quad (27)$$

because this integral has support from a triangle in the $(\sin \alpha, \phi)$ plane (see Fig. 1c) (it is a triangle only in the limit $n \rightarrow \infty$ of course).

From Eq. (23) one can deduce that the base length (in the ϕ direction) and the height (in the $\sin \alpha$ direction) of this triangle scale as $1/n$. A short calculation now yields that $J_n \sim 1/n^{2-\tau/2}$. Differentiation gives $j_n \sim 1/n^{3-\tau/2}$. The fact that $l_{\mathbf{q}} \sim n$ together with Eq. (24) implies that the $a_{\mathbf{q}}$'s decay as $\sim 1/n^{3-3\tau/2}$. The density of accessible disks is uniform in Δ (since they lie along the corridors), so our final result is

$$p(\Delta) \sim \frac{1}{\Delta^{3-3\tau/2}} \quad \Delta \gg \frac{1}{2R} \quad (28)$$

This power law does not depend on the small- R limit.

Next we assume that Eq. (28) holds whenever $\Delta > 1/2R$. The prefactor of Eq. (28) is then determined by demanding that $p_{\tau}(\Delta)$ is continuous at $\Delta = 1/2R$. In order to get correct normalization for $\tau = 0$ we multiply the entire $p_{\tau}(\Delta)$ by $(\pi/3)^2$ and we arrive at Eq. (19). This approximation crudely neglects the transitional behavior above $\Delta = 1/2R$. The error thus induced will be discussed in Section 3.4, but the present approximation will be very handy for estimating the Lyapunov exponent.

As a check we compute the mean laminar length $\langle \Delta \rangle$ in the distribution (19) with $\tau = 0$, which is found to be $\langle \Delta \rangle = 1/2R$, which indeed agrees with the small- R limit of the exact result $\langle \Delta \rangle = 1/2R - \pi R/2$.⁽¹⁹⁾

3.2. Lyapunov Exponents

The approximate zeta function we are going to work with is obtained by inserting Eq. (19) into Eq. (18). The power-law tail of $p(\mathcal{A})$ implies that the leading zero $k=0$ of the zeta function is also a branch point and the integral (18) diverges in the half-plane $\text{Im}(k) > 0$. As the asymptotics of the trace depend on the vicinity of the leading zero, we need the analytic continuation of the zeta function into the upper half-plane. We will achieve this by means of the (generalized) series expansion around the branch point $z=0$, which is straightforward since the zeta function may be expressed in terms of standard functions

$$\hat{Z}_\tau(k) \approx 1 - \frac{4}{3} \frac{\Gamma((2-\tau)/2)^2}{\Gamma(2-\tau)} \frac{R^{-2\tau}}{2^{1+\tau}} \times \left[z^{-1-\tau} \gamma(\tau+1, z) + z^{2-3\tau/2} \Gamma\left(-2 + \frac{3\tau}{2}, z\right) \right] \quad (29)$$

where $z = ik/2R$. The functions $\gamma(a, z)$ and $\Gamma(a, z)$ are incomplete gamma functions.⁽²⁰⁾

Expanding this to first order in τ gives

$$Z = \left\{ z + \frac{z^2}{3} \left(\log z + \gamma - \frac{11}{6} \right) \dots \right\} + \left\{ \left[-\frac{7}{12} + \log(2R^2) \right] + \left[\frac{11}{6} + \log(2R^2) \right] z \dots \right\} \tau \dots \quad (30)$$

The derivation of this expansion is rather lengthy, but the only step that is slightly tricky is the expansion of the incomplete gamma function $\Gamma(a, z)$ near an integral power a . We have for convenience thrown away all indices of the zeta function and use the strict equality sign, but we must not forget that we work with an approximation of an approximation of the exact zeta function.

We must now proceed with some care, since the leading zero is not isolated; a branch cut along the negative real z -axis reaches all the way up to it (we have chosen the principal branch of the logarithm).

We are interested in the following derivative of the trace [cf. Eq. (8)]

$$\begin{aligned} \frac{d}{d\tau} \text{tr } \mathcal{L}^\tau &= \frac{d}{d\tau} \frac{1}{2\pi i} \int e^{-z\tau} \frac{d}{dz} \log Z \, dz \Big|_{\tau=0} \\ &= \frac{1}{2\pi i} \int e^{-z\tau} \frac{d}{d\tau} \frac{d}{dz} \log Z \Big|_{\tau=0} dz \end{aligned} \quad (31)$$

where we have differentiated inside the integral sign (this step, although trivial, is a key step). We have now formulated Eq. (6) in the rescaled and rotated z -plane using rescaled time $t' = 2Rt$. The function to be Fourier transformed is

$$\begin{aligned} & \frac{d}{d\tau} \frac{d}{dz} \log Z|_{\tau=0} \\ &= \left[\frac{7}{12} - \log(2R^2) \right] \frac{1 + (z/3)(2 \log z + 2\gamma - 5/6) \dots}{z + (z^2/3)(\log z + \gamma - 11/6)^2 \dots} \\ &= \left[\frac{7}{12} - \log(2R^2) \right] \left(\frac{1}{z^2} + \frac{1}{3z} \dots \right) \end{aligned} \tag{32}$$

where we have kept only those terms yielding the leading term and the first correction. Collecting it all together yields

$$\lambda = \lim_{t \rightarrow \infty} 2R \left[\frac{7}{12} - \log(2R^2) \right] \left(1 + \frac{1}{6Rt} \dots \right) = 2R \left[\frac{7}{12} - \log(2R^2) \right] \tag{33}$$

The limiting value is due to the behavior of the zero [Eq. (9) is indeed valid], but the power-law correction is due to the fact that it sits on a branch point. The particular size of the first correction is not very accurate, as we will realize after Sections 3.4 and 3.5 (see also Appendix), but we just note in passing that there exist slowly decaying corrections indicating slow convergence of the Lyapunov exponent in numerical computations.

In Fig. 2 we compare numerical results on the Lyapunov exponent with our expression $\lambda = 2R[\frac{7}{12} - \log(2R^2)]$. The numerical values, from ref. 21, are calculated for rather large disk radii, where we should not expect much agreement *a priori*. Nevertheless our estimate is only 5% wrong when $R = 0.1$. The reason why the numerical values exceed our estimates for large R is easily understood. This is because the disk faces (in the unfolded system) come closer to each other, so that taking the length of the relevant lattice vector (as we did) overestimates the time of flight between them.

The Lyapunov exponent of the corresponding Poincaré map with the disk defining the SOS is related to the Lyapunov exponent of the flow according to⁽²²⁾

$$\lambda_{\text{map}} = \lambda \langle \mathcal{A}_s \rangle \approx \lambda/2R \approx \left[\frac{7}{12} - \log(2R^2) \right]$$

We see that $\lambda_{\text{map}} \rightarrow -2 \log(R) + 7/12 - \log 2$ when $R \rightarrow 0$, which agrees with the conjectured limit^(23, 24) $\lambda_{\text{map}} = -2 \log(R) + C + O(R)$. Indeed we have found an estimate of the constant $C \approx 7/12 - \log 2 \approx -0.110$. This is

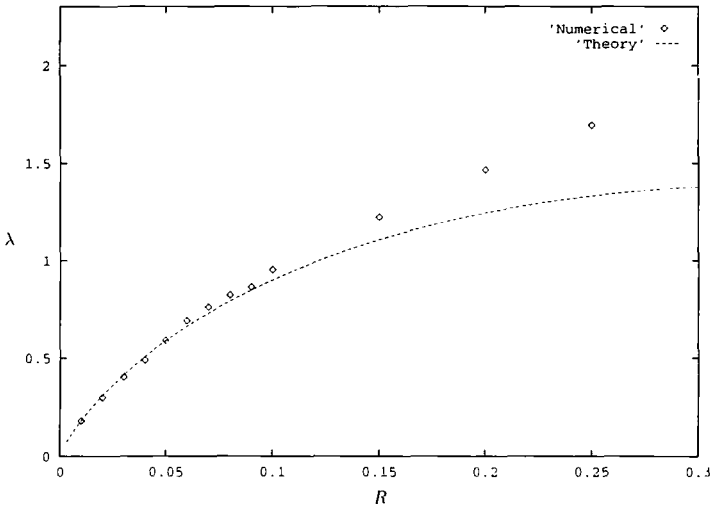


Fig. 2. Lyapunov exponent versus disk radius according to numerical simulation and Eq. (33).

very close to the numerical value found by ref. 23, as far as we can extract it from Fig. 2 in ref. 23. Refinement of this estimate amounts to refinement of the expression for $p(\Delta)$; we will return to this problem in future work. The smallness of the fudge factor $(3/\pi)^2$ used at the end of Section 3.1 indicates why the error seems so small.

Most theoretical work on the small- R limit of the Lyapunov exponent or Kolmogorov–Sinai entropy tries to verify the term $-2 \log R$,^(23,25) and few authors attack the problem of computing C . The constant C has been computed in ref. 26 for the related problem where the disks in the Lorentz gas are distributed randomly in the plane. The authors found that in this case the constant is $C = 1 - \log 2 - \gamma \approx -0.27036$ (with the same units and density of disks as in our case).

Although our zeta function is only expected to work at the immediate vicinity of $k = 0$, we cannot resist the temptation of using Eq. (19) to compute the generalized Lyapunov exponents. In Fig. 3 we plot the generalized Lyapunov exponents thus obtained for different disk radii. Note that when $\tau > 0$ the leading zero is indeed isolated and we do not have to worry about the cut. The position of the zero is computed numerically.

The quantity $\lambda(1)$ is the topological entropy, which tends to a finite limit when $R \rightarrow 0$. If we, as in Fig. 3, use Eq. (19), it is easy to show that $\lambda(1) \rightarrow (4\pi/3)^{1/2} \approx 2.0466$, as this depends only on the small- Δ limit of $p_{\tau=1}(\Delta)$. However, because of this, we can avoid the fudge factor and use

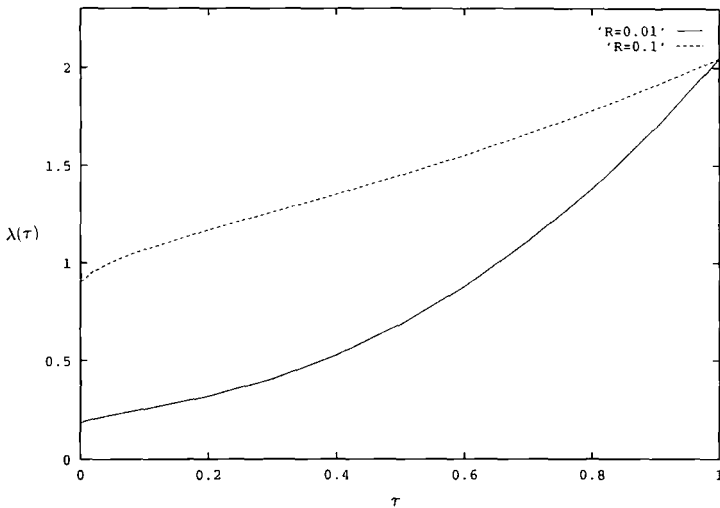


Fig. 3. Generalized Lyapunov exponents $\lambda(\tau)$ versus τ for two disk radii.

Eq. (25) instead and obtain $\lambda(1) \rightarrow (12/\pi)^{1/2} \approx 1.95441$, which is Berry's estimate.⁽²⁷⁾ However, the exact small- R limit is $\lambda(1) \rightarrow 1.9133307629\dots$ ⁽⁹⁾ The reason for the error in Berry's estimate is purely number-theoretic—our approximation was expected to work around $k=0$ and down in the complex plane the zeta function depends also on the correction to the mean density of coprimes.

When $\tau < 0$ the branch cut itself will provide the leading behavior of the trace—a power law,^(9, 14) and the generalized Lyapunov exponent will be zero. This means that $\lambda(\tau)$ cannot be analytic at $\tau=0$. This is referred to as a phase transition.⁽¹¹⁾

3.3. A First Calculation of the Diffusion Constant

We now turn to the computation of the diffusion constant. We will arrive at our final result in a roundabout way. We start with the coarse description of Section 3.1 and then carefully investigate what details need to be improved.

We calculate the generalized probability distribution $p_w(\Delta)$ using appropriate weight (13). We keep only the spatial components of β yielding the two-dimensional vector $\mathbf{\beta}$. As we study smeared $p_{\mathbf{\beta}}(\Delta)$, it suffices to approximate the spatial part of $(\hat{f}^t(x) - x)$ with the lattice vector \mathbf{q} . So, we must now compute the generalized probability distribution $p_{\mathbf{\beta}}(\Delta)$ à la Section 3.1, but using the weight $\exp(\mathbf{\beta} \cdot \mathbf{q}) = \exp[\beta q \cos(\phi_{\beta} - \phi_q)]$, where we

have written $\mathbf{q} = q(\cos(\phi_q), \sin(\phi_q))$ and $\mathbf{\beta} = \beta(\cos(\phi_\beta), \sin(\phi_\beta))$. We can use the result of Section 3.1 to some extent, since we realize, after inspecting Eq. (17), that we can make the following factorization:

$$p_\beta(\Delta) = p_0(\Delta) \frac{\int e^{\Delta\beta \cos(\phi_q - \phi_\beta)} d\phi_q}{\int d\phi_q} \tag{34}$$

In order to find the support of this integral we need to know the angular distribution of accessible disks for a particular value of $q = \Delta$. To this end we introduce the following simplifying assumptions

1. The coprime lattice points are distributed isotropically.
2. If $q > 1/2R$, we assume only four corridors with ϕ_q equal to one of $0, \pi/2, \pi,$ or $3\pi/2$.

Assumption 2 means a rather brute neglect of the transitional behavior at $\Delta \approx 1/2R$. We neglect the important fact the number of corridors grows when $R \rightarrow 0$. We comment on this in Section 3.5. The important thing now is that we preserve the symmetry in order to prevent net drift.

We first consider the case $q < 1/2R$. Using assumption 1 above gives

$$\begin{aligned} p_\beta(\Delta) &= \frac{4}{3} R \frac{1}{2\pi} \int_0^{2\pi} e^{\beta\Delta \cos \phi} d\phi \\ &= \frac{4}{3} RI_0(\beta\Delta) \\ &= \frac{4}{3} R \left(1 + \frac{\beta^2\Delta^2}{4} \dots \right), \quad \Delta < \frac{1}{2R} \end{aligned} \tag{35}$$

where I_0 is a modified Bessel function. In order to calculate the zeta function we need the Fourier transform of this,

$$\int_0^{1/2R} p_\beta(\Delta) e^{-ik\Delta} d\Delta = \frac{2}{3} \left(1 - \frac{z}{2} + \frac{z^2}{6} \dots \right) + \frac{\beta'^2}{6} \left(\frac{1}{3} - \frac{z}{4} + \frac{z^2}{10} \dots \right) \dots \tag{36}$$

where we have used rescaled variables $z = ik/2R$ and $\beta' = \beta/2R$.

Next we consider the limit $q > 1/2R$. We find, using the second assumption above,

$$p_\beta(\Delta) = \frac{2}{3(2R)^2} \frac{1}{\Delta^3} (e^{\beta'_x\Delta} + e^{-\beta'_x\Delta} + e^{\beta'_y\Delta} + e^{-\beta'_y\Delta}), \quad \Delta > \frac{1}{2R} \tag{37}$$

Fourier transforming this gives

$$\int_{1/2R}^{\infty} p_{\mathbf{p}}(\Delta) e^{-ik\Delta} d\Delta = \frac{1}{6} [E_3(z - \beta'_x) + E_3(z + \beta'_x) + E_3(z - \beta'_y) + E_3(z + \beta'_y)] \quad (38)$$

The resulting zeta function can now be expanded

$$\begin{aligned} Z_{\mathbf{p}} &= 1 - \int_0^{\infty} p_{\mathbf{p}}(\Delta) e^{-ik\Delta} d\Delta \\ &= \frac{1}{6} (\gamma - \frac{11}{6}) \beta'^2 + z(1 - \frac{1}{3} \beta'^2) + z^2 \frac{1}{3} (\gamma - \frac{11}{6}) \\ &\quad + \frac{1}{12} [(z - \beta'_x)^2 \log(z - \beta'_x) + (z + \beta'_x)^2 \log(z + \beta'_x) \\ &\quad + (z - \beta'_y)^2 \log(z - \beta'_y) + (z + \beta'_y)^2 \log(z + \beta'_y)] \dots \end{aligned} \quad (39)$$

According to Section 2.2, we are interested in the following quantity:

$$\begin{aligned} &\left(\frac{\partial^2}{\partial \beta_x^2} + \frac{\partial^2}{\partial \beta_y^2} \right) \text{tr } \mathcal{L}' |_{\beta' = 0} \\ &= \left(\frac{\partial^2}{\partial \beta_x^2} + \frac{\partial^2}{\partial \beta_y^2} \right) \frac{1}{2\pi i} \int e^{z't'} \frac{d}{dz} \log Z dz |_{\beta = 0} \\ &= \frac{1}{(2R)^2} \frac{1}{2\pi i} \int e^{z't'} \left(\frac{\partial^2}{\partial \beta_x'^2} + \frac{\partial^2}{\partial \beta_y'^2} \right) \frac{d}{dz} \log Z |_{\beta = 0} dz \end{aligned} \quad (40)$$

We now proceed in the same way as in Section 3.2. We want to determine the asymptotic behavior of the Fourier transform of

$$\left(\frac{\partial^2}{\partial \beta_x'^2} + \frac{\partial^2}{\partial \beta_y'^2} \right) \frac{d}{dz} \log Z |_{\beta = 0} \sim \frac{2}{3z^2} \left(\frac{4}{3} - \log z - \gamma \right) \quad (41)$$

To this end we now need the integral

$$\frac{1}{2\pi i} \int \frac{\log z}{z^2} e^{z't'} dz = t'(1 - \gamma - \log t') \quad (42)$$

In deriving this it is convenient to use contour integration and let the contour encircle the negative real z axis. We thus find the following diverging diffusion constant [$D = \lim_{t \rightarrow \infty} D(t)$]:

$$D(t) = \frac{1}{2t} \left(\frac{\partial^2}{\partial \beta_x^2} + \frac{\partial^2}{\partial \beta_y^2} \right) \text{tr } \mathcal{L}' |_{\beta' = 0} = \frac{1}{18R} [1 + 3 \log(2Rt)] \quad (43)$$

This logarithmic divergence of the diffusion constant agrees with ref. 13, but the prefactor is not correct. The computation will be refined in Section 3.5. The important thing to learn from this section is that the Laplacian exposes the logarithm in the series expansion of the zeta function. So we now know where to focus our attention, namely at the tail of $p_{\beta}(\Delta)$.

3.4. A Closer Look at the Tail

At the end of Section 3.1 we aimed at finding a good approximation for $p_{\tau}(\Delta)$ for the whole range $1/2R < \Delta < \infty$. This was convenient for the calculation of the Lyapunov exponent, which depends on the integral $\int p_{\tau}(\Delta) d\Delta$ for small τ , and we thus needed a uniform approximation to $p_{\tau}(\Delta)$. But the diffusion constant depends only on the $\Delta \rightarrow \infty$ behavior of $p(\Delta)$.

In this section we restrict ourselves to the case $\tau = 0$ and will compute the limit $\lim_{\Delta \rightarrow \infty} \Delta^3 p_0(\Delta)$.

Let us look at the corridor with direction vector $\mathbf{q} = (n_x, n_y)$, where n_x and n_y are coprime. Suppose for a moment that \mathbf{q} lies in the first octant, so that n_x and n_y are positive and $n_x \geq n_y$. The accessible disks in this corridor are the ones labeled $\mathbf{q}' + n\mathbf{q}$ and $\mathbf{q}'' + n\mathbf{q}$, where \mathbf{q}' and \mathbf{q}'' are the predecessor and successor in the Farey sequence of order n_x (see Fig. 1 and recall the definition of Farey sequences,⁽¹⁸⁾ see also Section 3.2 in ref. 9; the statement above should appear obvious). A calculation analogous to the one at the end of Section 3.1 now gives the following expression for $a_{\mathbf{q}}(0)$ [as defined in Eq. (24)]:

$$a_{\mathbf{q}' + n\mathbf{q}}(0) = \frac{1}{2\pi} \frac{2qR + 1/(2qR) - 2}{q^2 n^3} + O\left(\frac{1}{n^4}\right) \tag{44}$$

and the same holds for the sequence $\mathbf{q}'' + n\mathbf{q}$. The contribution to $p_0(\Delta)$ is

$$\sum_n a_{\mathbf{q}' + n\mathbf{q}}(0) \delta(\Delta - |q' + nq|) = \frac{1}{\Delta^3} \frac{1}{2\pi} \left(2qR + \frac{1}{2qR} - 2 \right) \tag{45}$$

To compute the tail of $p_0(\Delta)$ we need to sum over all coprime \mathbf{q} such that $q < 1/2R$. We restrict the summation to the first quadrant $\mathbf{q} \in S$:

$$S = \{ \mathbf{q} = (n_x, n_y) \mid n_y > 0; n_x \geq 0; (n_x, n_y) = 1; (n_x^2 + n_y^2) < 1/2R \} \tag{46}$$

and multiply the result by four, to account for all four quadrants, and then by two, to account for both \mathbf{q}' and \mathbf{q}'' defined above. The result is

$$p_0(\Delta) \sim \frac{4}{\pi\Delta^3} \sigma(R) + O\left(\frac{1}{\Delta^4}\right) \tag{47}$$

where

$$\sigma(R) = \sum_{\mathbf{q} \in S} \left(2qR + \frac{1}{2qR} - 2 \right) \tag{48}$$

The $R \rightarrow 0$ limit of $\sigma(R)$ is given in ref. 13: $\sigma(R) = (1/4\pi R^2)[1 + O(R^{1/4})]$.

Let us expand the unweighted zeta function Z_0 into the more general series

$$Z_0 = \sum_{i=1}^{\infty} a_i z^i + \sum_{i=2}^{\infty} b_i z^i \log z \tag{49}$$

For the approximation of $p_0(\Delta)$ worked out in Section 3.1 we have $b_i = 0$ for $i \geq 3$. The correct value of b_2 may be computed from Eq. (47) (using, e.g., standard expansions of exponential integrals) and is found to be $b_2(R) = 8R^2\sigma(R)/\pi$ and the small- R limit is $b_2 \rightarrow 2/\pi^2$, which differs considerably from the result in Section 3.1. The reason for this error is the neglect of a smooth transition at $\Delta = 1/2R$ in Eq. (19). This crossover behavior is indeed slow, as is indicated from the $O(1/\Delta^4)$ term above. Generally we expect the asymptotics of the tail to look like $p(\Delta) \sim \sum_{n \geq 3} c_n/\Delta^n$, so that there may exist nonzero b_i of any order.

3.5. A Second Calculation of the Diffusion Constant

One might suspect that the coarse assumptions, especially assumption 2 in Section 3.3, could give rise to an error in the prefactor of superdiffusion. We will now demonstrate that the prefactor is robust against refinements of this assumption. A better estimate of $p_\beta(\Delta)$ is obtained by replacing $\exp(\beta'_x \Delta) = \exp[\beta' \Delta \cos(\phi_\beta)]$ in Eq. (37) with the averaged quantity

$$\frac{1}{2c\Delta} \int_{-c/\Delta}^{c/\Delta} e^{\beta' \Delta \cos(\phi_\beta - \phi_q)} d\phi_q \tag{50}$$

The integration range decreases like $1/\beta$, since the width of the corridor is constant. For sufficiently large Δ we can take $\beta' \cos(\phi_\beta - \phi) \approx \beta'_x + \beta'_y \phi$ and find that the integral above is

$$e^{\beta'_x \Delta} [1 + O(\beta'^2_y)] \tag{51}$$

The correction is $O(\beta'^2)$ and has no effect on $D(t)$, as anticipated.

In the considerations in Section 3.3 we also reduced the number of corridors to four. Or, more precisely, we bunched together all corridors into these four, but ensured that the correct Z_0 was recovered when $\beta_x = \beta_y = 0$. In doing this we destroy all angular information about the diffusion, but the size of diffusion is left unaffected, as is easily realized by studying how the Laplacian acts on (39).

We are led to the conclusion that the prefactor of superdiffusion depends solely on the coefficient b_2 of the unweighted zeta function (49) according to $D(t) = (b_2/2R) \log t$. Inserting the correct value of b_2 from the previous section, we arrive at

$$D(t) = \frac{4R\sigma(R)}{\pi} \log t \rightarrow \frac{1}{R\pi^2} \log t, \quad R \rightarrow 0 \quad (52)$$

which is indeed the suggested exact result.⁽¹³⁾

Again there are slowly decaying corrections to $D(t)$ and it is not surprising that the numerical detection of this diffusion law has eluded serious attempts.⁽²⁸⁾

4. CONCLUDING REMARKS

The main advantage of the approximation outlined in this paper is its apparent simplicity. It is far easier to apply than a proper cycle expansion would be, taking all the (infinite number of) pruning rules into account, and it gives a very good description of the leading zero. If one persists in a periodic orbit approach, one has to realize that the slow convergence of the leading zero reflects the nature of the singularity at the origin and this singularity carries information about the dynamics in which we are interested.

Apart from the excursion down in the complex k -plane when computing generalized Lyapunov exponents, our interest in this paper has been restricted to the behavior of the zeta functions around the origin $k=0$ or equivalently the coarse structure of the traces. We could thus work out a very coarse description of $p(\Delta)$. In ref. 9 we demonstrated that refinement of the expression for $p(\Delta)$ down to a scale $\sim R$ leads to a good description of the trace down to this scale. In order to probe finer scales, e.g., to study semiclassical spectra, one has to find corrections to the BER method. To this end it might be useful to try to combine periodic orbit techniques with the asymptotic knowledge of zeta functions and traces obtained from the BER method.

The major drawback of the BER approximation is the lack of an error term; so far we have no bounds on the errors in our computations. It is of course highly desirable to work out such bounds, which would put the present considerations on mathematically firm ground.

APPENDIX

Here we derive Eq. (3). Notations used are defined in Section 2.1. The approach is inspired by ref. 29.

First we expand the invariant density $\rho(x)$ into a sum over periodic orbits. The invariant density is obtained as the following time average:

$$\rho(x) = \lim_{\varepsilon \rightarrow 0} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \delta_\varepsilon(x - f^t(x_0)) dt \quad (\text{A1})$$

where ε is a small smearing width. If $\varepsilon = 0$, this is true for almost all x_0 , but x_0 must not lie on a periodic orbit. But as long as $\varepsilon \neq 0$ we can safely put $x_0 = x$, irrespective of whether it is a periodic point or not, and get

$$\rho(x) = \lim_{\varepsilon \rightarrow 0} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \delta_\varepsilon(x - f^t(x)) dt \quad (\text{A2})$$

The next few steps are yet not rigorously verified except for a very restricted class of systems,⁽²⁹⁾ but the result is believed to hold for a much bigger class. We differentiate with respect to T and interchange the limits $\varepsilon \rightarrow 0$ and $T \rightarrow \infty$ and get

$$\rho(x) = \lim_{T \rightarrow \infty} \delta(x - f^T(x)) = \lim_{T \rightarrow \infty} \int \delta(y - f^T(y)) \delta(x - y) dy \quad (\text{A3})$$

The integral has support from periodic points only. We split the integration variable y according to $dy = dy_\perp + dy_\parallel$, where y_\perp is perpendicular to the flow and y_\parallel is parallel. We perform the integration and get

$$\rho(x) = \lim_{T \rightarrow \infty} \sum_{p \in \text{p.p.o.}} \sum_{n=1}^{\infty} \frac{\delta(T - nT_p)}{|\det(1 - M_p^n)|} \int_{y \in p} \delta(x - y) \frac{dy_\parallel}{v(y)} \quad (\text{A4})$$

where $v(y)$ is the speed at y .

The expectation value can now be expressed in terms of periodic orbits and we arrive at Eq. (3)

$$\lim_{t \rightarrow \infty} \langle w \rangle = \lim_{t \rightarrow \infty} \int w(x, t) \rho(x) dx \tag{A5}$$

$$= \lim_{t \rightarrow \infty} \sum_{p \in \text{p.p.o.}} T_p \sum_{n=1}^{\infty} w_p^n \frac{\delta(t - nT_p)}{|\det(1 - M_p^n)|} \tag{A6}$$

where we have used the fact the weight is constant along a periodic orbit so

$$\int_{y \in p} w(y, t) dy_{||}/v = w(y_p, t) \int dy_{||}/v = w(y_p, t) T_p$$

where y_p is any point on a primitive periodic orbit p . The multiplicative property of the weight finally implies $w(y_p, t) = w(y_p, T_p)^n \equiv w_p^n$.

After having established the final expressions, one should provide the remaining delta functions with a small width.

In Eq. (A6) we let t and T approach the asymptotic limit together, $T=t$. We can thus only extract the leading asymptotic behavior of $\langle w(x, t) \rangle$. This is because the normalization $\int \rho(x) dx$ can approach unity rather slowly. In the Sinai billiard we have $\int \rho(x) dx \rightarrow 1 - C(R)/t$, as can be verified by the methods described in this paper.

If one wants to rigorously verify Eq. (A6) for the Sinai billiard, one has to deal with the presence of marginally stable orbits. However, these form a set of zero measure in phase space and subtraction of this set from Eq. (2) does not affect the result, so we do not consider this as any problem.

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