Cycle averaging formulas applied to a periodic Lorentz gas

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Abstract

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The diffusion constant and the Lyapunov exponent for the spatially periodic Lorentz gas are evaluated numerically in terms of periodic orbits. A symbolic description of the dynamics reduced to a fundamental domain is used to generate the shortest periodic orbits. Applied to a dilute Lorentz gas with finite horizon, the theory works well, but for the dense Lorentz gas the convergence is hampered by the strong pruning of the admissible orbits.

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CHAOS, AND WHAT TO DO ABOUT IT

course project, spring semester 2014

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I. INTRODUCTION

[34] The Lorentz gas [2] is one of the simplest nontrivial models of deterministic diffusion. Diffusion of a light molecule in a gas of heavy scatterers is modelled by a point particle in a plane bouncing off an array of reflecting disks. As a billiard built up completely of concave surfaces and as a pure hyperbolic system, the Lorentz gas is a good candidate for description in terms of cycle expansions [3]. This might seem a hopeless task, as one has to deal with all periodic and aperiodic solutions of an infinitely extended system. An approach based on larger and larger finite portions of the system is described in ref. [4], with the diffusion constant related to the escape rates from such finite portions. As far as escape rates are obtained in direct numerical simulations this approach has been shown to be effective [5]. However, from the cyclists point of view where the rates are calculated from the periodic orbits, this approach is impractical; with each added disk new peculiarities arise in the enumeration of periodic orbits, and with current methods there is little hope of getting results for more than a few disks, and no hope of approaching the desired scaling limit.

A recent approach, introduced in ref. [6] and tested in this paper, exploits the fact that the periodic Lorentz gas can be constructed by putting together translated copies of an elementary cell. Therefore quantities characterizing global dynamics, such as the Lyapunov exponent and the diffusion constant, can be computed from the dynamics restricted to the elementary cell.

II. THE PERIODIC LORENTZ GAS

In the periodic Lorentz gas [2] a point particle reflects elastically off a periodic array of reflecting disks in a plane. The system can be thought of as an unfolding of the Sinai billiard [7]. The

[32] Pavel 2014-04-18: a footnote
[33] Tingnan 2014-04-18: a footnote
[34] Predrag: the initial text from Cvitanović, Gaspard and Schreiber [1]

standard diffusion constant can be defined if the particle has a bounded free path between any two successive bounces. An example is a triangular array with sufficiently small inter-disk spacing. Unfortunately, as we shall see, the same mechanism that guarantees a finite horizon also leads to rather awkward pruning of periodic orbits.

Machta and Zwanzig [8] have given numerical results for the diffusion constant in Lorentz gases, as well as estimates based on a random walk approximation. We shall follow their notation and fix the radius of the disks to 1, assume unit particle speed, and denote the spacing between the disks by w (see fig. 1). The horizon is finite for $w < 4/\sqrt{3} - 2 = 0.3094\ldots$.

III. DIFFUSION

In this section we briefly review the derivation of a formula for the diffusion coefficient of a spatially periodic system in terms of the periodic orbits in an elementary cell, originally given in ref. [6] (which contains a more detailed treatment together with considerations about the discrete symmetries and a reduction of the dynamics to a fundamental domain).

The method applies to any hyperbolic dynamical system that is a periodic tiling $\widehat{M} = \bigcup_{\hat{n}\in T} M_{\hat{n}}$ of the dynamical phase space $\widehat{M}$ by translates $M_{\hat{n}}$ of an *elementary cell* M, with T the Abelian group of lattice translations.

It is convenient to define two time evolution operators, one for the whole phase space, and one for the elementary cell. Let $\hat{x}_t = \hat{\phi}^t(\hat{x})$ denote the point in the global space $\widehat{M}$ obtained by the flow in time t, and $x_t = \phi^t(x)$ denotes the corresponding flow in the elementary cell. The two are related by

$$\hat{n}_t(x) = \hat{\phi}^t(x) - \phi^t(x) \in T \ , \tag{1}$$

the translation of the endpoint of the global path into the elementary cell M.

Given a fixed vector $\beta \in \mathbf{R}^d$, where d is the dimension of the phase space, one can extract the diffusive properties of the Lorentz gas from the generating function

$$\langle e^{\beta\cdot(\hat{x}_t - x)} \rangle \ , \tag{2}$$

where the average is over all $x \in M$.

The diffusive properties follow by studying

$$Q(\beta) = \lim_{t\to\infty} \frac{1}{t} \log\langle e^{\beta\cdot(\hat{x}_t - x)} \rangle \tag{3}$$

and its derivatives at $\beta = 0$. Clearly $Q(0) = 0$, and if by symmetry all odd derivatives vanish (i.e. there is no drift), the second derivatives

$$\frac{\partial}{\partial\beta_i}\frac{\partial}{\partial\beta_j}Q(\beta)\Big|_{\beta=0} = \lim_{t\to\infty}\frac{1}{t}\langle(\hat{x}_t - x)_i(\hat{x}_t - x)_j\rangle \ , \tag{4}$$

yield a (generally anisotropic) diffusion matrix. The spatial diffusion constant is then given by

$$D = \frac{1}{2\nu}\sum_{i=1}^{\nu}\frac{\partial^2}{\partial\beta^2}Q(\beta)\Big|_{\beta=0} = \lim_{t\to\infty}\frac{1}{2t}\langle(\hat{q}_t - q)^2\rangle \ , \tag{5}$$

where the i sum is restricted to the ν spatial components q_i of the phase space vectors x.

The basic ingredient of this approach is the reduction of the average (3) to the elementary cell. In order to understand this recall that (3) can be written as

$$\langle e^{\beta\cdot(\hat{x}_t - x)}\rangle = \int_{\substack{x\in M\\ \hat{y}\in\widehat{M}}} dxd\hat{y}e^{\beta\cdot(\hat{y}-x)}\mathrm{Prob}_t(x\to\hat{y} \tag{6}$$

$$= \frac{1}{|M|}\int_{\substack{x\in M\\ \hat{y}\in\widehat{M}}} dxd\hat{y}e^{\beta\cdot(\hat{y}-x)}\delta(\hat{y} - \hat{\phi}^t(x)) \ . \tag{7}$$

Here, $|M| = \int_M dx$ is the volume of the elementary cell M. Note that there is a unique lattice translation $\hat{n}$ such that $\hat{y} = y - \hat{n}$, with $y \in M$. Now the translational invariance can be used to reduce the integral over y to the elementary cell:

$$\langle e^{\beta\cdot(\hat{x}_t - x)}\rangle = \frac{1}{|M|}\int_{x,y\in M} dxdye^{\beta\cdot(\hat{\phi}^t(x)-x)}\delta(y - \phi^t(x)) \ . \tag{8}$$

In this way the global $\hat{\phi}^t$ flow averages can be computed by following the flow ϕ^t restricted to the elementary cell M. As is well known [9], the $t\to\infty$ limit of such averages can be recovered by means of transfer operators. The eq. (8) suggests that we study the operator $\mathcal{L}^t$ whose kernel is given by

$$\mathcal{L}^t(y,x) = e^{\beta\cdot(\hat{x}_t - x)}\delta(y - x_t) \ , \tag{9}$$

where $\hat{x}_t = \hat{\phi}^t(x) \in \widehat{M}$, but $x, x_t, y \in M$. It is straightforward to check that this operator has the semigroup property, $\int_M dz\mathcal{L}^{t_2}(y,z)\mathcal{L}^{t_1}(z,x) = \mathcal{L}^{t_2+t_1}(y,x)$. The quantity of interest (3) is given by the leading eigenvalue of $\mathcal{L}^t$, $\lambda_0 = e^{tQ(\beta)}$. In particular, for $\beta = 0$, the operator (9) is the Perron-Frobenius operator, with the leading eigenvalue $\lambda_0 = 1$ (the probability conservation).

To evaluate the spectrum of $\mathcal{L}$, consider

$$\mathrm{tr}\,\mathcal{L}^t = \int_M dxe^{\beta\cdot\hat{n}_t(x)}\delta(x - x_t) \ . \tag{10}$$

Here $\hat{n}_t(x)$ is the discrete lattice translation defined in (1). For discrete time and hyperbolic dynamics we have

$$\mathrm{tr}\,\mathcal{L}^t = \sum_{\substack{p:\tau_p r=t,\\ r\in\mathbf{N}}} \sum_{x\in p} \frac{e^{\beta\cdot\hat{n}_t(x)}}{|\det\left(\mathbf{1}-\mathbf{J}^r(x)\right)|}\ , \tag{11}$$

where the sum is over periodic points of all prime cycles p whose period τ_p divides t, and $\mathbf{J}_p(x) = D\phi^{\tau_p}(x)$. Note that the sum over cycle points of p can be replaced by a factor τ_p, as $\det(\mathbf{1}-\mathbf{J}_p) = \det(\mathbf{1}-\mathbf{J}_p(x))$ and $\hat{n}_p = \hat{n}_{\tau_p}(x)$ are independent of x. For the Jacobian $\mathbf{J}_p$ this follows by the chain rule, and for the travelled distance $\hat{n}_p$ this follows by continuing the path periodically in $\widehat{M}$. For the discrete time case we finally obtain

$$\det(1-z\mathcal{L}) = \prod_p \exp\left(-\sum_{r=1}^{\infty}\frac{z^{\tau_p r}}{r}\frac{e^{r\beta\cdot\hat{n}_p}}{|\det\left(\mathbf{1}-\mathbf{J}_p^r\right)|}\right)\ , \tag{12}$$

where the product runs over the set $\mathbf{P}$ of prime cycles.

Generalization to continuous time [10, 11] amounts to the replacement $z^{\tau_p}\to e^{-s\tau_p}$, where τ_p is now the (not necessarily integer) period of the prime cycle p:

$$Z(\beta,s) = \prod_{p\in\mathbf{P}} \exp\left(-\sum_{r=1}^{\infty}\frac{1}{r}\frac{e^{(\beta\cdot\hat{n}_p-s\tau_p)r}}{|\det\left(\mathbf{1}-\mathbf{J}_p^r\right)|}\right)\ . \tag{13}$$

The associated Ruelle zeta function is then (see e.g. ref. [3] for details)

$$1/\zeta(\beta,s) = \prod_{p\in\mathbf{P}}\left(1-\frac{e^{\beta\cdot\hat{n}_p-s\tau_p}}{|\Lambda_p|}\right)\ , \tag{14}$$

with $\Lambda_p = \prod_e \lambda_{p,e}$ the product of the expanding eigenvalues of $\mathbf{J}_p$.

The first main result of ref. [6] is that the function $Q(\beta)$ of eq. (3) is the largest solution of the equation $Z(\beta,Q(\beta))=0$ (or equivalently, of $1/\zeta(\beta,Q(\beta))=0$).

The above infinite products can be rearranged as expansions with improved convergence properties [3]. To present the result, we define $t_p = e^{\beta\cdot\hat{n}_p-s\tau_p}/|\Lambda_p|$, and expand the zeta function (14) as a formal power series,

$$\prod_{p\in\mathbf{P}}(1-t_p) = 1 + {\sum_{p_1,\ldots,p_k}}' t_{\{p_1,\ldots,p_k\}}\ , \tag{15}$$

where

$$t_{\{p_1,\ldots,p_k\}} = (-1)^k t_{p_1}t_{p_2}\cdots t_{p_k}\ , \tag{16}$$

and the sum is over all distinct non-repeating combinations of prime cycles. Taking two derivatives, as in the derivation of eq. (35) and eq. (80) in ref. [3] one obtains the main formula tested numerically in this paper:

The diffusion constant (5) is given by

$$D = \frac{1}{2\nu} \frac{\sum'(-1)^k(\hat{n}_{p_1} + \cdots + \hat{n}_{p_k})^2/|\Lambda_{p_1} \cdots \Lambda_{p_k}|}{\sum'(-1)^k(\tau_{p_1} + \cdots + \tau_{p_k})/|\Lambda_{p_1} \cdots \Lambda_{p_k}|} \ , \tag{17}$$

with sums as in (15). The beauty of this formula is that even though the global trajectory is in general not periodic, $\hat{n}_p \neq 0$, the reduction to the elementary cell enables us to compute the desired quantity in the usual way, in terms of periodic orbits.

Apart from the diffusion constant we will compute Lyapunov exponents and test the probability conservation. Because it involves derivatives of zeta functions the formula for the largest Lyapunov exponent takes a similar form as the one for the diffusion constant above (17). The formula (modified for continuous time) is given in ref. [3], eq. (91):

$$\lambda = \frac{\sum'(-1)^k(\mu_{p_1} + \cdots + \mu_{p_k})/|\Lambda_{p_1} \cdots \Lambda_{p_k}|}{\sum'(-1)^k(\tau_{p_1} + \cdots + \tau_{p_k})/|\Lambda_{p_1} \cdots \Lambda_{p_k}|} \ . \tag{18}$$

In this formula $\mu_p = \ln|\Lambda_p|$ denotes the stability exponent of a cycle. Note that all quantities involved here are invariant under the symmetries of the lattice.

A. A simple example: A chain of Baker's maps

Some confidence can be gained at this point by applying the above formula (17) to a trivial system, a chain of coupled baker maps studied in ref. [12]. In this case there are only four fixed points, all with stability $\Lambda_p = 1/2$, two of which give rise to the translations $\hat{n}_p = \pm 1$. As the system is uniformly hyperbolic, all curvature terms are identically zero, and the fixed points substituted into (17) yield immediately the correct result $D = 1/4$.

IV. DYNAMICS IN THE ELEMENTARY CELL

Unfolding a periodic orbit in the elementary cell can result either in a closed orbit in the whole lattice or in a segment of some translational movement. According to the above result (17) the diffusive properties of the system follow from the relation between the closed and the translating orbits.

Since the system is closed the escape rate is zero. Therefore the dynamical zeta function (eq. (14) with $\beta = 0$) should have its first zero at $z = 1$. $\zeta(0,0)$ is simply $1 + \sum'(-1)^k/|\Lambda_{p_1} \cdots \Lambda_{p_k}|$.

The periodic orbits in the elementary cell can be found in a systematic way. Starting at a given disk, the trajectory can reach any of the neighboring twelve disks in the next bounce. A symbolic dynamics is obtained by labelling these displacements anticlockwise with numbers 0 to 11. When 0 denotes a flight between disks which are nearest neighbors all even numbers do so. For any spacing there is an obvious pruning rule that motion in the same direction cannot be repeated twice in a row because the particle cannot cross a disk. In fact, for the dense gas considered here, the direction has to change at least by two units after each bounce. After a long flight (odd label) the change has to be at least 3.

The cycles corresponding to a given symbol sequence can now be found e.g. by minimizing the length of a path visiting the disks according to the symbols.

Although the discrete C_{6v} symmetry of the elementary cell is not exploited in the diffusion formula, it can be used to reduce the necessary computational effort. The images of a cycle under rotation and reflection do not have to be computed separately. Nevertheless the huge number of symbols drastically restricts the maximal cycle length attainable in numerical calculations.

Table 1 shows the results obtained for a spacing of $w = 0.3$. Note that because of the pruning rule there cannot be a fixed point with these symbols.

As mentioned above a lot of orbits turn out to be forbidden when the required finite horizon is achieved by making the spacing between disks small enough. This is immediately reflected in the fact that the number of orbits does not increase by a factor of eleven each time the length is increased. Indeed, for the cycles computed so far, the average factor is less than four. So very poor convergence of cycle expansions has to be expected. With this in mind the numbers given in table I are in a reasonable accord with the probability conservation and also not a disaster for the Lyapunov exponent (compare with the more accurate estimates of table 5). Nevertheless, the estimates of the diffusion constant up to the number of cycles employed so far do not show any convergence at all. They seem to be more sensitive to the bad shadowing than the Lyapunov exponent and the probability conservation.

A. Dilute Lorentz gas

In order to test the diffusion formula under less trying conditions, we eliminate pruning by making the spacing between disks larger, and imposing the finite horizon by fiat; in this section we consider the measure zero subset of those orbits which after each bounce travel only to one of the

nearest or next nearest disks. This set is a Cantor set repeller, and the probability is not conserved. Estimates of the Lyapunov exponent and the diffusion constant for trajectories restricted to this set are given in table 2.

As the set is not the full set of orbits contributing to diffusion, there are no results obtained by other means that these numbers could be compared with. Encouragingly, the diffusion constant exhibits reasonable convergence, supporting the claim that the cycle expansion formula is in principle convergent, but for high density of scatterers the convergence is adversely affected by the strong pruning of the allowed orbits.

V. REDUCTION TO THE FUNDAMENTAL DOMAIN

In ref. [6] some effort is made to derive a diffusion formula similar to (17) involving quantities within the fundamental domain. The fact that lattice translations do not commute with the symmetry group within the elementary cell makes this apparently a difficult and not yet completed task. Therefore only results for the Lyapunov exponent (18) and the probability conservation are given in this section.

The fundamental domain symbolic dynamics used here, due to F. Christiansen (unpublished), is given in figs. 3, 4 and table II. Now the symbols indicate relative direction changes instead of the absolute directions. The right and left turns are not distinguished - instead, one reads off a symbol whether the next turn has to be taken in the same or in the opposite sense. Lower case letters denote short flights between close-by disks, upper case denotes the long flights to the next nearest disks. Each symbol corresponds to a given relative change in direction. The exact amount of change depends on whether the last flight was long (odd label in the notation of the last section) or short (even label). Table II give the definition of the symbols.

Christiansen had originally proposed to denote symbols 'f' and 'F' by the same letter, thus reducing the size of the alphabet. We prefer to use instead the two letters together with the pruning rule that 'f' can only follow an uppercase letter (i.e. a long segment) and 'F' only a lowercase letter. The symbols given to an orbit by this scheme are invariant under all spatial symmetries of the system but not under the time reversal.

Of the possible twelve symbols, 'A', 'B', 'f' and 'F' are pruned as soon as the horizon gets finite. Among the remaining symbols there is still strong pruning, reflected in the fact that for $w = 0.3$ the number of cycles of symbol length n does not grow like 8^n but roughly as 3^n. Figure 5 shows

all the fundamental domain fixed points which are not pruned at $w = 0.3$ together with an example of a pruned fixed point.

Table 4 gives some impression of the pruning involved. In order that longer orbits be shadowed by shorter ones, for every combination of two symbols a two-cycle, and the fixed points corresponding to each of the symbols should exist. Two-cycles such as 'ac', 'aC', ... are missing while corresponding "shadowing" pseudo-cycles 'a c', 'a C' exist, and conversely, two-cycles occur where one of the symbols has no corresponding fixed point (e.g. the symbol 'd' in 'ad'). So shadowing seems to be largely dysfunctional, at least as long as finite approximate Markov partitions are not developed. With this in mind the convergence which can be seen in table 5 is better than expected. Furthermore, for general reasons discussed in ref. [13], the convergence of cycle expansions for dynamics restricted to the fundamental domain is considerably better than for the elementary cell, as can be verified by comparing the Lyapunov exponent and probability conservation estimates in the two cases.

To conclude, we have tested numerically the recently proposed formula for deterministic diffusion in the Lorentz gas. While the cycle expansions work well in estimating the more traditional indicators of deterministic chaos, such as the Lyapunov exponent, they do not yet lead to converging estimates of the diffusion constant for the dense Lorentz gas. This appears to be a consequence of the severe symbolic dynamics pruning and the attendant lack of shadowing in cycle expansions. Whether this difficulty can be surmounted by more careful control of the symbolic dynamics remains to be seen.

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length	# cycles	λ	D
1	0	-	-
2	54	0.5528	1.6716
3	440	0.5588	1.7006
4	3234	0.5604	1.7054
5	27856	0.5605	1.7049

Table 2: Elementary cell, w=2.0, imposed finite horizon

		a	b	c	d	e	C	D	E
	1	x	x	x			x	x	
a	x	-	x		x				
b	x	x	-	x	x	x			x
c	x		x	-	x	x		x	
d		x	x	x	-			x	
e			x	x		-			
C	x						-		
D	x			x	x			-	
E			x						-

Table 4: Problematic shadowing, w=0.3

length	# cycles	$\zeta(0,0)$	λ
1	5	-1.216975	-
2	10	-0.024823	1.745407
3	32	-0.021694	1.719617
4	104	0.000329	1.743494
5	351	0.002527	1.760581
6	1243	0.000034	1.756546

Table 5: Fundamental domain, w=0.3

. FLOTSAM, REMOVED FROM REF. [6]

A. Reduction from $\widehat{M}$ to $\widetilde{M}$

To deal with the continuous time problem in the fundamental domain, it is convenient to view the flows $\tilde{\phi}$, ϕ, and $\hat{\phi}$ as suspensions [Bo] by successive disk collision times τ of maps $\tilde{f}$, f, and $\hat{f}$, mapping respectively $\widetilde{\Omega}$, Ω, and $\widehat{\Omega}$ onto themselves. Here the fundamental domain phase space is now

$$\widetilde{\Omega} \;=\; [0, \pi/6] \times [-\pi/2, \pi/2] \;,$$

with the first coordinate the impact position, and the second coordinate the impact angle on the disc. The elementary cell phase space is then $\Omega \;=\; \tilde{\Omega} \times G$, and the full domain phase space is $\widehat{\Omega} \;=\; \Omega \times T$, where G is the discrete symmetry group, and T is the translation group of the lattice. We can write $x \in \Omega$ uniquely as

$$x \;=\; g \circ \tilde{x} \equiv (\tilde{x}, g) \;,$$

with $\tilde{x} \in \widetilde{\Omega}$ and $g \in G$. The action of f in this representation is

$$f(\tilde{x}, g) \;=\; (\tilde{f}(\tilde{x}), \gamma(\tilde{x}, g)) \;,$$

with the composition law

$$\gamma(f^2(\tilde{x}, g)) \;=\; \gamma(\tilde{f}(\tilde{x}), \gamma(\tilde{x}, g)) \;=\; \gamma(\tilde{f}(\tilde{x}), 1) \cdot \gamma(\tilde{x}, 1) \cdot g \;.$$

The (vectorial) distance which a particle travels up to the next disc-collision in $\widehat{M}$ when starting at $\tilde{x} \in \widetilde{\Omega}$ is denoted by $n(\tilde{x})$, and it is a vector in $\mathbf{R}^2$. The length of $n(\tilde{x})$ is proportional to $\tau(\tilde{x})$. When the starting point is at $(\tilde{x}, g)$, then

$$n(\tilde{x}, g) \;=\; g \circ n(\tilde{x}, 1) \;=\; g \circ n(\tilde{x}) \;.$$

Assume now that $\tilde{x}$ is a periodic point for $\tilde{f}$, of period $r|\tilde{p}|$: $\tilde{f}^r(\tilde{x}) = \tilde{x}$. The time to run around this periodic orbit is (DEFINE periodic points):

$$\sigma_{\tilde{p}} = \sum_{j=0}^{|\tilde{p}|-1} \tau(\tilde{x}_{\tilde{p},j}) \;.$$

If we fix $g \in G$ then the distance covered (in $\widehat{M}$) when starting at $(\tilde{x}, g)$ is

$$n(\tilde{x}, g, r) \;=\; \sum_{j=0}^{r-1} n(\tilde{f}^j(\tilde{x}), \gamma(f^j(\tilde{x}, g))) \;=\; \sum_{j=0}^{r-1} \gamma(f^j(\tilde{x}, g)) \circ n(\tilde{f}^j(\tilde{x})) \;.$$

This can be transformed further by using the composition law for γ:

$$n(\tilde{x}, g, r) \;=\; g \circ n(\tilde{x}, 1, r) \;=\; \sum_{j=0}^{r-1} \gamma(f^j(\tilde{x}, 1)) \cdot \gamma(f^{j-1}(\tilde{x}, 1)) \cdot \ldots \cdot \gamma(\tilde{x}, 1) \circ n(\tilde{f}^j(\tilde{x}), 1) \; .$$

The ζ function is now defined [Ru] by

$$\zeta(\beta, s) \;=\; \exp \sum_{r=1}^{\infty} \frac{1}{r} \sum_{\tilde{x} \in \mathrm{Fix} \tilde{f}^r} \sum_{g \in G} \exp \left(\beta \cdot n(\tilde{x}, g, r) - sr\sigma_{\tilde{p}} \right) \; .$$

Define now

$$N(\tilde{x}, g) \;=\; \lim_{m \to \infty} m^{-1} n(\tilde{x}, g, m \cdot \rho) \; ,$$

where $\rho = \rho(\tilde{x})$ is the minimal period of $\tilde{x}$.

This function exists, and satisfies

$$N(\tilde{x}, g) \;=\; g \circ N(\tilde{x}, 1) \; .$$

Note that we also have

$$\begin{aligned} N(f^j(\tilde{x}, g)) \;&=\; N(\tilde{f}^j(\tilde{x}), \gamma(f^j(\tilde{x}, g)) \\ &=\; N(\tilde{f}^j(\tilde{x}), \gamma(f^j(\tilde{x}, 1) g) \\ &=\; g \circ N(\tilde{f}^j(\tilde{x}), \gamma(f^j(\tilde{x}, 1))) \\ &=\; g \circ N_j(\tilde{x}) \; , \end{aligned} \tag{19}$$

where we define

$$N_j(\tilde{x}) \;=\; N(f^j(\tilde{x}, 1)) \; .$$

Similarly, the time for multiple runs on the same cycle is additive and we define

$$\tau_j(\tilde{x}) \;=\; \tau(\tilde{f}(\tilde{x})) \; .$$

We define now a new zeta function by

$$\zeta_0(\beta, s) \;=\; \exp \sum_{r=1}^{\infty} \frac{1}{r} \sum_{\tilde{x} \in \mathrm{Fix} \tilde{f}^r} \sum_{g \in G} \exp \sum_{j=0}^{r-1} \left(g^{-1} \circ \beta \cdot \frac{r}{\rho(\tilde{x})} N_j(\tilde{x}) - s\tau_j(\tilde{x}) \right) \; ,$$

and in terms of prime cycles we get

$$\frac{1}{\zeta_0(\beta, s)} \;=\; \prod_{\tilde{p} \in \tilde{\mathcal{P}}} \prod_{g \in G} \left(1 - \frac{\exp \sum_{j=0}^{r_{\tilde{p}}-1} \left\{ g^{-1} \circ \beta \cdot N_j(\tilde{x}) - s\tau_j(\tilde{x}) \right\}}{|\Lambda_{\tilde{p}}|} \right) \; ,$$

where $r_{\tilde{p}}$ is the period of $\tilde{p}$, $\tilde{x}$ is any point on $\tilde{p}$, and $\Lambda_{\tilde{p}}$ is the product of the expanding eigenvalues. Let us denote

$$L(\tilde{p}) \;=\; \sum_{j=0}^{r_{\tilde{p}}-1} N_j(\tilde{x}) \;,$$

and

$$T(\tilde{p}) \;=\; \sum_{j=0}^{r_{\tilde{p}}-1} \tau_j(\tilde{x}) \;.$$

The second derivative of ζ_0 w.r.t. β still contains the operation of the group...? Rearranging the series, one gets now

$$D \;=\; \frac{1}{2}\frac{\sum'(-1)^k \left(\sum_{\ell=1}^k \sum_{g\in G} g\circ L(\tilde{p}_\ell)\right)^2 / |\Lambda_{\tilde{p}_1}\cdots\Lambda_{\tilde{p}_k}|}{\sum'(-1)^k |G| \left(\sum_{\ell=1}^k T(\tilde{p}_\ell)\right) / |\Lambda_{\tilde{p}_1}\cdots\Lambda_{\tilde{p}_k}|} \;.$$

Probably pulling a character out of the CEsym paper eliminates all terms except those in which both g's are equal in the square...?

REMARK on boundary orbits

B. DESYMMETRIZATION

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from predrag/articles/diffus/dif12.tex, stuff thrown out by Gaspard 18 oct 93

Reduction of periodic orbit formulas from M to the fundamental domain $\widetilde{M}$ is convenient for practical calculations, because desymmetrization improves considerably the convergence of cycle expansions. Reduction of G to its irreducible representations leads to the factorization of (**??**) into a product of irreducible subspace determinants. To make this factorization more transparent, we illustrate it first by the simple example of the case of inversion symmetry $\sigma x \;=\; -x$, with M tiled by $\widetilde{M} \cup -\widetilde{M}$, and $\mathcal{L}$ of the form

$$\mathcal{L}(y,x) \;=\; e^{\beta\cdot\hat{f}(x)}\delta(y-f(x)) \;,$$

where both $\hat{f}$ and f commute with inversion, $f(-x) = -f(x)$. We rewrite $\mathcal{L}$ as

$$\begin{aligned}\mathcal{L}(y,x) \;&=\; \tfrac{1}{2}e^{\beta\cdot\hat{f}(x)}\left(\delta(y-f(x)) + \delta(-y-f(x))\right) \\ &\quad + \tfrac{1}{2}e^{\beta\cdot\hat{f}(x)}\left(\delta(y-f(x)) - \delta(-y-f(x))\right) \\ &= \mathcal{L}_+ + \mathcal{L}_- \;,\end{aligned}$$

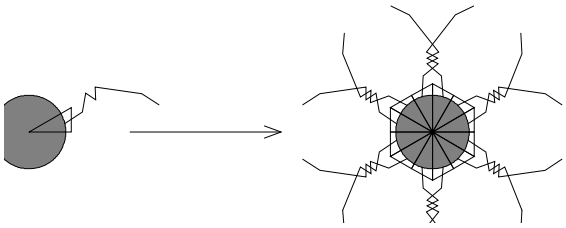

FIG. 1: $h_{\tilde{p}}$ is the discrete transformation that relates the endpoint of the cycle $\tilde{p} \in \widetilde{M}$ to the endpoint of the corresponding trajectory segment in M. Eckmann [6] Fig. 2. Remember to include schreiberFig2.tex

(20)

with $\mathcal{L}_+$ and $\mathcal{L}_-$ denoting the symmetric and the antisymmetric parts, respectively. Now $\mathrm{tr}\,\mathcal{L} = \mathrm{tr}\,\mathcal{L}_+ + \mathrm{tr}\,\mathcal{L}_-$, and

$$\mathrm{tr}\,\mathcal{L}_\pm = \int_{\widetilde{M}} d\tilde{x} \sum_{g=1,\sigma} e^{(g\beta)\cdot\hat{f}(\tilde{x})} \frac{1}{2} \sum_{h=1,\sigma} \chi_\pm(h)\delta(h\tilde{x} - f(\tilde{x})) \,,$$

where χ is the representation character, $\chi_\pm(1) = 1$, $\chi_\pm(\sigma) = \pm 1$.

The generalization of (**??**) to an arbitrary finite group [CE2, Ro] is now

$$\begin{aligned} \mathrm{tr}\,\mathcal{L}^t &= \sum_{\alpha\in\mathcal{I}_G} \mathrm{tr}\,\mathcal{L}^t_\alpha \\ \mathrm{tr}\,\mathcal{L}^t_\alpha &= \sum_{\substack{\tilde{p}:\sigma_{\tilde{p}}r=t,\\ r\in\mathbf{N}}} \frac{\chi_\alpha(h^r_{\tilde{p}})}{|\det\left(\mathbf{1} - \tilde{\mathbf{J}}^r_{\tilde{p}}\right)|} \sum_{\tilde{x}\in\tilde{p}} \frac{1}{|G|} \sum_{g\in G} e^{(g\beta)\cdot(\hat{f}^t(\tilde{x})-\tilde{x})} \,, \end{aligned} \tag{21}$$

where α runs over the irreducible representations of G, χ_α is the character of the representation α, and $\tilde{p}$ is a prime cycle in $\widetilde{M}$. $h_{\tilde{p}}$ is defined as in figure 1: Let p be a lift of the cycle $\tilde{p}$ to M, choosing any initial point on $\tilde{p}$. If the orbit ends in $\widetilde{M}'$, then $h_{\tilde{p}}$ is defined by $h_{\tilde{p}}\widetilde{M} = \widetilde{M}'$. The (orthogonal) matrix $\mathbf{H}_{\tilde{p}}$, the derivative of the action of $h_{\tilde{p}}$ on M, $h_{\tilde{p}} \circ x = \mathbf{H}_{\tilde{p}}x$, is absorbed into the definition of the fundamental domain Jacobian, $\tilde{\mathbf{J}}_{\tilde{p}} \equiv \mathbf{H}^{-1}_{\tilde{p}}\mathbf{J}_{\tilde{p}}$. If $\tilde{p}$ is on the boundary of $\widetilde{M}$, the above formula needs a further modification – for details see refs. [La, CE2].

. FIGURE CAPTIONS

Figure 2 A portion of a chaotic trajectory with about 300 bounces is shown. Although the particle is often trapped between neighboring disks for several bounces, there are also segment of the trajectory which take the particle over a large distance with few bounces.

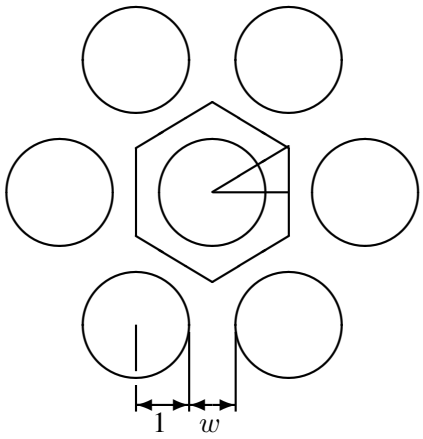

FIG. 2: A small portion of a triangular Lorentz gas. The whole set of scatterers can be obtained by translating the elementary cell indicated in the figure.

Figure 3 The upper row shows the case when the preceding segment has been a long one, the lower row the case when it has been a short one. The arrows at the end points indicate the sense of the next change of direction. Due to the discrete symmetry of the triangular lattice, all translated, rotated or reflected copies of each situation shown are denoted by the same symbol.

Figure 4 The upper row shows the case when the preceding segment has been a short one, the lower row the case when it has been a long one.

Figure 5 Shown are global orbits which reduce to fixed points in the fundamental domain. Five of them (a,b,c,C,D) are not pruned for $w = 0.3$, the spacing shown here. The sixth (B) is an example of a pruned cycle; it exists for a dilute Lorentz gas, because for the dense Lorentz gas its trajectory is blocked by the center disk. Both B and D denote turns by 120 degrees, but D also changes the sense of rotation at each bounce.

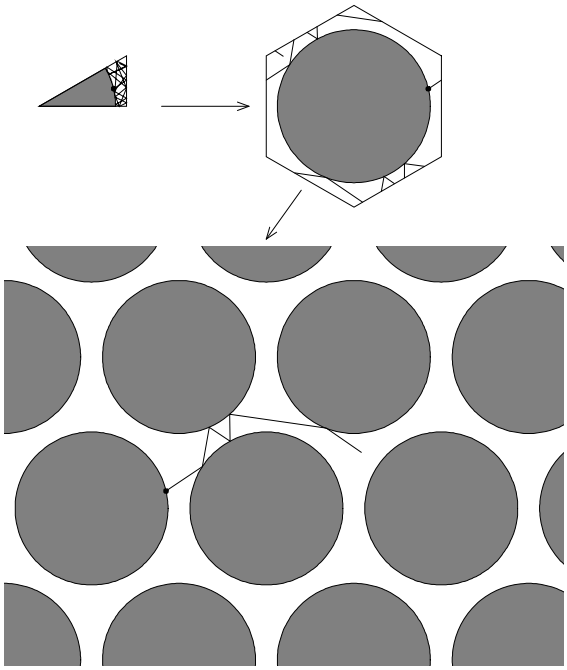

FIG. 3: Eckmann [6] Fig. 1, from dif15.pdf. Remember to include (misnamed) schreiberFig1.tex

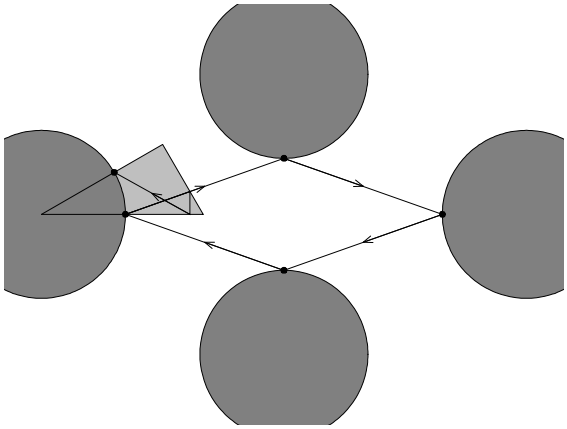

FIG. 4: Eckmann [6] Fig. 3. Remember to include schreiberFig3.tex

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. DAILY BLOG

2013-02-03 Roberto incorporate kneading determinants from G. Cristadoro [14] *Fractal diffusion coefficient from dynamical zeta functions*.

2009-02-27 Predrag Read Gilbert and Lefevere [15], "Heat conductivity from molecular chaos hypothesis in locally confined billiard systems,"

"From Deterministic Chaos to Deterministic Diffusion" by R. Klages,

arXiv:0804.3068: " A set of easy-to-read lecture notes for a short first-year Ph.D. student course. The notes cover five hours of lectures and do not require any prior knowledge on dynamical systems. The first part introduces to deterministic chaos in one-dimensional maps in form of Lyapunov exponents and the metric entropy. The second part first outlines the concept of deterministic diffusion. Then the escape rate formalism for deterministic diffusion, which expresses the diffusion coefficient in terms of the above two chaos quantities, is worked out for a simple map. The notes conclude with a very brief sketch of anomalous diffusion.

For 'fundamental domain' in hyperbolic geometry, see for example these notes by Kimball Martin.

2014-02-27 Predrag Must read: Dettmann [16], *Diffusion in the Lorentz gas*.

generate `f_diff_MarkPart.pdf` from `.../xfig/f_diff_MarkPart.fig`

2013-02-28 Predrag to Tingnan Zhang: Dettmann's review,

arXiv:1402.7010 is something that you want to read - looks very complete. **Goldman:** Sects. 7.4 and 7.5 and refs within are tantalizing.

2013-03-25 Predrag to Tingnan Zhang: *Superdiffusion in the periodic Lorentz gas* by Jens Marklof and Balint Toth,

arXiv:1403.6024 is too mathematical and general for our purposes (hopefully we will have no super-diffusivity, noise should wipe that out), but Sect. 2 *The scattering map* might be useful for your exposition (or its prequel

arXiv:0801.0612).

2014-04-18 Predrag Sinai [17] might be a quick read. Recent references of possible interest: Zhang [18] *Current in periodic Lorentz gases with twists*.

2014-04-18 Predrag I have saved the Lorentz [2] 1905 *The motion of electrons in metallic bodies* (click here).

2014-04-18 Predrag For great wallpapers, see overheads in Engel's course.

2014-04-18 Predrag Dresselhaus *et al.* textbook [19] (click here) is good on discrete and space (but not continuous) groups. The MIT course 6.734 online version contains much of the same material.

Chapter *9. Space Groups in Real Space* is quite clear on matrix representation of space groups. The translation group T is a normal subgroup of G and defines the Bravais lattice. The cosets by translation T (set all all group elements obtained by all translations) form a factor group G/T, isomorphic to the point group g (rotations). All irreducible representations of G can be compounded from irreducible representations of g and T.

Section *9.3 Two-Dimensional Space Groups*: In the international crystallographic notation, our hexagonal lattice #17 is called $p6mm$, with point group $6mm$.

$$g = \{E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}\}$$

Prefix p indicates that the unit cell is primitive (not centered). This is a simple or *symmorphic* group, which makes calculations easier. The Bravais lattice is two equilateral triangles, not sure how to relate it to our hexagonal 'elementary cell'? A Brilloun zone? Bravais 'unit cell' is illustrated in Fig. E.2. ChaosBook 'Fundamental domain' makes an appearance in Fig. 10.2.

The main trick in quantum-mechanical calculations is to go to the *reciprocal* space (see Fig. E.2), in our case with the full Γ point, $k = 0$, wave vector symmetry (see Table 10.1), and 'Large Representations'. This is something we have not tried in deriving the trace formula for deterministic diffusion.

Sect. *10.5 Characters for the Equivalence Representation* look like those for the point group, sort of. We should probably work out problems 10.1 and 10.2.

2014-04-24 Tingnan Remember that some orbits that lie on the boundary of fundamental domain have only 6 copies.

2014-04-26 Predrag All divisors of 12 are possible multiplicites. The fully symmetric state of multiplicity 1 would be an equilibrium point at the origin: possible for soft potentials but not for this billiard. Rest you can easily doodle if you draw the hexagonal lattice (disks replaced by point): there is periodic orbit of length 6 (edges of the hexagon) of multiplicity 2 (the two orientations of the orbit), and there should be orbits of multiplicity 3, 4, 6 and the generic asymmetric orbits of multiplicity 12.

2014-04-24 Pavel Tingan and I have realized that in a pseudo-cycle it is possible to have two or more prime cycles that differ by a group action. In some sense, cross-terms still disappear, but it is impossible to assign unique weights to each fundamental domain cycle.

2014-04-26 Predrag to Tingan After the project is delivered, have a look at Knauf [20, 21], *Ergodic and topological properties of Coulombic periodic potentials*, *Motion in periodic potentials*, Baldwin [22] *Soft billiard systems*, Kimball [23] *Chaotic properties of the soft-disk Lorentz gas*, Bálint and Tóth [24, 25] *Correlation decay in certain soft billiards*, *Mixing and its rate in 'soft' and 'hard' billiards motivated by the Lorentz process*, and Elyutin [26] *Lyapunov exponent for a gas of soft scatterers*. Blog about relevant parts here, if there is something of interest to us.

2014-04-26 Predrag We should read Chapter 7 of Gaspard [27]. Kimberly and I both have a hard copy. Gaspard discusses irreps of the translation group in some detail.

2014-04-26 Predrag I'm quite convinced that this problem is a solved problem, we just have to understand how characters are used to project irreps of space groups. One has to go to the reciprocal lattice, and utilize utilize the concept of the 'star'. All physical chemists and crystallographers know how to do this - we just need to be good students and read the stuff. Our case is the most symmetric, $p6mm$ lattice - it is surely worked out in some paper in a way that we can understand. They call our 'fundamental domain' the 'motif' or the 'asymmetric unit'.

I found projects in this course easy to read, especially Tomaž Čendak, who reviews the space groups theory in a pretty simple way, and Zavadlav has very pretty wallpaper groups illustrations. Ziherl recommends Elliott and Dawber, *Symmetry in Physics* [28].

Joseph Sidighi likes Cotton [29] *Chemical applications of group theory*, which has no characters for space groups, but a very pretty discussion of their geometry in Chapt. 11. Cotton was "the most influential inorganic chemist to ever have lived."

You can write up the projects either together, starting with this file, with all stuff that does not belong to the public version bracketed by `ifboyscout...fi` . I think that would be a good learning experience for both of you. Or separately, as two projects. In that case, add them to this folder, `reducesymm/tingnan/` as separate files. You can clip & paste anything from here or from ChaosBook.org, if that saves you LaTeXing time.

If we succeed in factorization, this would merit a publication. It is OK if you do not succeed in factorization - I have failed myself, so who am I to cast the first stone:)

2014-05-02 Predrag Pavel again has an idea. Forget the translation group; tile every Lorentz gas orbit by the little triangles (copies of the fundamental domain, 1/12th of the elementary cell). Then the group orbit is generated by 3 elements (ignoring going through the corners): go to the domain to the left/right (generators of D_{12}) and flip the domain so it leaves the elementary cell. To Predrag this is reminiscent of Penrose tailings, where the space is tiled without the translations over square or cubic lattice. For that, Mermin's article [30] on space groups of quasicrystals might be of interest.

I think the idea should be worked out in one dimension first, but Pavel thinks that would be too simple. Predrag believes that you always work out the simplest model first. $\Lambda = 2$ vanishes by eq. (25.20) (click here), so the simplest diffusion models are for $\Lambda = 3$ or 4. Reduce the map to the fundamental domain (positive 1/2 line) as in ChaosBook fig. 9.8: The bimodal Ulam sawtooth map (click here). That should give the symmetry-reduced symbolic dynamics, but the group is larger than D_1, which works 'within the elementary cell', by generating the negative axis copy of the fundamental domain: one adds a reflection that flips the flips the fundamental domain (the half-unit interval) outside of the elementary cell, to the adjoining tile (the second one to the left or the right. This operation generates the translations, and together the two group operations assign a symbolic itinerary to any orbit. Then one should find the rule that reads of the global translation from the symbolic itinerary, insert this into the cycle expansions for the deterministic diffusion formula.

For $\Lambda = 2$ I get that the fundamental domain dynamics is given by the full tent map (click here), so it cannot be simpler. Too bad that $D = 0$ identically :)

length	# cycles	$\zeta(0,0)$	λ	D
1	0	-	-	-
2	24	-0.31697	1.330	0.750
3	64	-0.54152	1.435	0.677
4	156	-0.09718	1.902	0.565
5	492	0.02383	2.324	0.425
6	1484	0.02812	1.931	0.259
7	5244	0.02044	1.836	0.371
8	19008	-0.00036	1.754	0.513
Ref. [8], estimate			-	0.175
numerical experiment			1.760	0.25

length	# cycles	$\zeta(0,0)$	λ	D
1	0	-	-	-
2	24	-0.34807	1.312	0.759
3	64	-0.57736	1.418	0.686
4	168	-0.11233	1.908	0.571
5	517	0.01373	2.406	0.407
6	1582	-0.01062	1.998	0.227
7	5387	-0.01084	1.900	0.333
8				
			?.???	?.???
numerical experiment				0.25

TABLE I: Elementary cell, w=0.3. (left) Schreiber 1992 calculation [1]. Gaspard 1992 note:: "My numerical estimate for the Lyapunov exponent when $w = 0.3$ is $\lambda = 1.760 \pm 0.002$, which supports the result of this table." (right) Zhang 2014-05-05 calculation.

2014-05-03 Predrag I drew by hand the D_1 reduction of the dynamics to the fundamental domain for $\Lambda = 3$ case - it is really simple and it works. Guys, try it, then try it for the Lorenz gas. I'm optimistic.

2014-05-03 Predrag Pavel is right - 1D case is probably misleading, I used only translations to find the global displacement. With reflections, the distances on the 2D lattice corresponding to relative prime cycles will not be integer vectors - their construction will resemble what we do when we bounce a straight trajectory off a sequence of 3-disks, it will be a computation, and go to the new 'comoving' coordinate frame. But a doable one. Maybe one should play with the least symmetric triangular $p3$ (C_3 point group) tiling first, rather than with the most symmetric hexagonal $p6mm$ lattice (D_6 point group).

2014-05-05 Tingnan My numbers of elementary cell prime cycles, Lyapunov exponents and diffusion coefficients are listed and compared to the Schreiber calculation in table I. I still have the problem for the convergence of diffusion coefficients. Did we miss a factor of 2 somewhere?

symbol	amount of change		direction of change	
	last long	last short	next the same	next other way
a	1	2	x	
b	3	4	x	
c	5	6	x	
d	5	4		x
e	3	2		x
f	1	-		x
A	2	1	x	
B	4	3	x	
C	6	5	x	
D	4	5		x
E	2	3		x
F	-	1		x

TABLE II: Symbols in the fundamental domain.

2014-05-07 Predrag Note that while Tingnan more prime periodic orbits than Thomas Schreiber, convergence is not improved. To the contrary: the diffusion constant and the Lyapunov exponent of table I do not agree for even $n = 2$, so something is seriously amiss. It is unlikely that Thomas and I would have gotten that wrong. Have to

1. Please create table III for the 24 cycles of length $n = 2$ with (a) symbolic dynamics (see Table II), (b) Λ_p, (c) T_p, and (d) $\hat{n}_t(x)$, the discrete lattice translation (1).
2. Check the Λ's, T's of the shortest ones, the ones that are the same as for the 3-disk billiard, against the analytical expressions given as exercises in ChaosBook, (click here).
3. Verify that Tingnan's implementations of (17) and (18) have been correctly coded.
4. table I

2014-05-05 Tingnan Figure 5 is taken from the Kimball article [23] on soft billiards. Let β_i and ϕ_i be the impact parameter and propagation angle(in the global frame) before i-th collision.

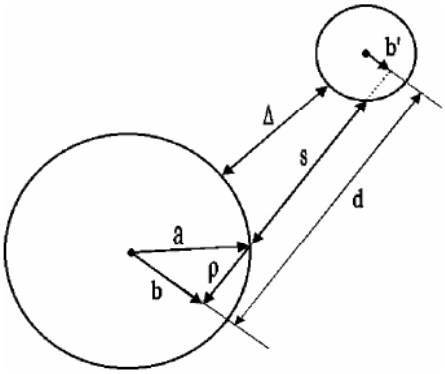

FIG. 5: A portion of a path;

We can then compute the monodromy matrix. Suppose the scattering funtion is provided by $\theta(b)$, we have: [35]

$$\phi_{j+1} = \phi_j + \theta_j(b_j);$$

[35] Predrag: 2014-05-05 promising start. Go on :)

TABLE III: All periodic orbits of topological length 2 (this table from ref. [31] to be used as a template). Listed are the topological length of the cycle, its expanding eigenvalue Λ's, its period T and its symbolic dynamics itinerary (see table II).

n_p	Λ_p	T_p	itinerary
2	$0.71516752438\times10^{1}$	0.6076252185107	0
2	$-0.29528463259\times10^{1}$	ALL FAKE NUMBERS	1
2	$-0.98989794855\times10^{1}$	0.3333333333333	10
2	$-0.13190727397\times10^{3}$	-0.2060113295833	100
2	$0.55896964996\times10^{2}$	0.5393446629166	110
2	$-0.10443010730\times10^{4}$	-0.8164965809277	1000
2	$0.57799826989\times10^{4}$	0.0000000000000	1100
2	$-0.10368832509\times10^{3}$	0.8164965809277	1110
2	$-0.76065343718\times10^{4}$	-1.4260322065792	10000
2	$0.44455240007\times10^{4}$	-0.6066540777738	11000
2	$0.77020248597\times10^{3}$	0.1513755016402	10100
2	$-0.71068835616\times10^{3}$	0.2484632276044	11100
2	$-0.58949885284\times10^{3}$	0.8706954728949	11010
2	$0.39099424812\times10^{3}$	1.0954854155465	11110
2	$-0.54574527060\times10^{5}$	-2.0341342556665	100000
2	$0.32222060985\times10^{5}$	-1.2152504370215	110000
2	$0.51376165109\times10^{4}$	-0.4506624359329	101000
2	$-0.47846146631\times10^{4}$	-0.3660254037844	111000
2	$-0.63939998436\times10^{4}$	0.3333333333333	110100
2	$-0.63939998436\times10^{4}$	0.3333333333333	101100
2	$0.39019387269\times10^{4}$	0.5485837703548	111100
2	$0.10949094597\times10^{4}$	1.1514633582661	111010
2	$-0.10433841694\times10^{4}$	1.3660254037844	111110