### TOPICS IN DYNAMICS: FIRST PASSAGE PROBABILITIES AND CHAOTIC PROPERTIES OF THE PHYSICAL WIND-TREE MODEL

A Dissertation Presented to The Academic Faculty

By

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### TOPICS IN DYNAMICS: FIRST PASSAGE PROBABILITIES AND CHAOTIC PROPERTIES OF THE PHYSICAL WIND-TREE MODEL

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#### **SUMMARY**

In chapter 2 we discuss finite time prediction for dynamical systems. Chapter 3 contains some basic results and examples concerning future efforts to extend the theorems of Chapter 2 to new contexts. Chapter 4 introduces the physical Wind-Tree model, proves that it is hyperbolic, and observes some of the new properties that it has compared to the classical Wind-Tree model.

# CHAPTER 1 INTRODUCTION

We begin by considering an example to motivate the theory presented in Chapter 1. This is followed by a brief historical introduction to the topic of Chapter 3. The subjects of chapters 1 and 3 are sufficiently distinct that it seems best to leave more detailed discussion of those topics to each of their respective chapters.

Consider the following autonomous system of differential equations, designed by Otto Rössler in 1976:

$$\frac{dx}{dt} = -y - z$$

$$\frac{dy}{dt} = x + ay$$

$$\frac{dz}{dt} = b + z(x - c).$$
(1.1)

These equations are useful in modeling equilibrium in chemical reactions. The solution to this system of equations is three functions: x(t), y(x), and z(t). We plot one solution to this problem numerically with a = 0.1, b = 0.1, c = 14, and  $0 \le t \le 150$ . The result is figure 1.1.

Any modern student of differential equations recognizes this as the appearance of chaos. Indeed, the Rössler equations have a so-called strange attractor as an invariant set. A typical means to understanding the behavior of such systems is to consider a return map on the attractor.

One picks a 2-dimensional plane and "cuts" the attractor. Given a point q in this intersection, let us denote the solution to equations (1.1) with initial condition q by q(t). Because of the recurrent nature of solutions, there is some moment in time t > 0 when q(t)again lies in the intersecting plane. One thus defines the return map  $\mathcal{F}(q) = q(t)$ .

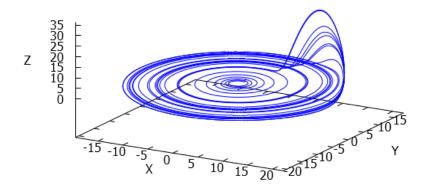


Figure 1.1: A typical solution to the Rössler equations

If one tracks the iterates  $q, \mathcal{F}(q), \mathcal{F}^2(q), \ldots$ , these points will trace out what appears to be a 1-dimensional curve C inside the intersecting plane. Indeed, if one describes a point q not by its spatial coordinates but by its arc-length location on C, then the return map  $\mathcal{F}$ takes the form of a unimodal map. That is, if S is the total arc length of C, then the return map  $\mathcal{F}$  can be expressed a function from [0, S] to itself that has a unique global maximum.

Already we have made some progress if our goal was to reduce the study of a solution to equations (1.1) to something more easily understood. However, we are most interested in predicting the exact behavior of solutions to these equations as well as possible.

Pick a point  $s, 0 \le s \le S$ . We define a binary sequence  $d_1 d_2 d_3 \dots$  as follows. Denote by m the point such that  $\mathcal{F}(m)$  is the maximum. Let  $d_i = 1$  if  $\mathcal{F}^i(s) > m$ , and  $d_i = 0$  if  $\mathcal{F}^i(s) < m$ .

This binary sequence "encodes" the entire future of a point s as it is moved around by  $\mathcal{F}$ . Consider the following very practical question: Given two subintervals  $I, J \subset [0, S]$ , can we predict which of these two subintervals the point s is most likely to enter first after n iterates of  $\mathcal{F}$ ? This is equivalent to asking if we can predict where the solution will be in three dimensional space at a certain moment in time. Such questions have been posed

about a variety of systems [1, 2, 3, 4, 5, 6].

We can divide the domain [0, S] up into subintervals such that s belongs to one of these subintervals if and only if  $d_1 \dots d_k = w_k \dots w_1$  where  $w_i \in \{0, 1\}$ . (The subinterval determines k and the values of each  $w_i$ ). So, to answer the asked question, we need to know how many binary sequences there are such that the following conditions are satisfied:

- $b_{n-k+1}\ldots b_n = w_k\ldots w_1$
- $b_i \dots b_{i+k-1} \neq w_k \dots w_1$  for every  $1 \le i \le n-k$ .

Note that the binary sequence representing s is infinitely long, but in order to answer the asked question it suffices to compare the number of strings of a fixed, finite length. This topic is explored in further depth, and with a greater explanation of the history regarding the subject, in Chapter 2. Chapter 3 contains some basic results and examples concerning future efforts to extend the theorems of Chapter 2 to new contexts.

The equations (1.1) are intended to provide a simple example of realistic behavior actually, to provide one of the simplest possible examples of certain behavior. Indeed, one cannot hope to find the chaotic behavior displayed by those equations in autonomous systems of differential equations in dimension less than 3. These equations are a "good" example, however, in that systems of more practical interest can be studied by similar means.

Broadly speaking, it is desirable to have a reserve of such examples. They should be as simple as possible, so as not to obfuscate the interesting phenomena. Phrased differently, the model should be only as complicated as necessary to display realistic behavior. Paul and Tatyana Ehrenfest were prolific sources of such interesting examples, publishing many well known and famous examples in their book [7].

Among the many was the Wind-Tree model, intended to be a "simplest possible" model of diffusion. One places rhombuses, called "trees", centered at each point of the integer lattice. One then considers the motion of a point particle (the "wind") as it travels through the plane, reflecting off the trees just as described for the diamond billiard.

The Wind-Tree model displayed some pathological behavior. It is not chaotic in the way that it was expected to be. In fact, the specific mathematical property that it lacked was hyperbolicity. Historically, this pathological behavior led to a preference for other "simplest possible" models which displayed more realistic phenomena, in particular the Lorentz gas. The Lorentz gas replaced the rhombuses with circles, and this change was sufficient to eliminate much of the pathology. This model has, in turn, been studied quite extensively (see Chapter 3 for a somewhat more detailed summary).

A simple change to the Wind-Tree model, however, will suffice to create the mathematical characteristics that were long sought in the original. If one merely replaces the point particle of the wind with a tiny circle, hyperbolicity is immediately obtained. We refer to the model so obtained as the physical Wind-Tree model. As discussed in Chapter 4, the study of statistical properties of the physical Wind-Tree model promises to be as rich as the study of the same properties for the Lorentz gas, if not more so.

#### **CHAPTER 2**

# WHERE AND WHEN ORBITS OF THE MOST CHAOTIC SYSTEMS PREFER TO GO

#### 2.1 Introduction

Dynamical systems theory was first created as a qualitative theory of ordinary differential equations. It appeared when the understanding came that generally one cannot solve differential equations analytically and thus obtain formulas  $x_t = f(x_0, t)$  which allow one to compute the state  $x_t$  of the system at any moment of time. Therefore a natural goal was to describe the behavior of solutions in the limit when time t tends to infinity. At first it was a local analysis mostly aimed at establishing stability for some simple (e.g. periodic) solutions. Then it was realized that the dynamics of many deterministic dynamical systems is intrinsically unstable. (Physicists refer to this type of phenomenon as the exponential divergence of initially close orbits or local exponential instability).

Thus the study of dynamical systems turned to probabilistic descriptions, an idea that can be traced back to the founding papers of Statistical Mechanics and especially to the notion of the ensemble introduced by Boltzmann.

In stochastic (probabilistic) systems, typical questions regard the existence of stationary distributions and the rates of convergence to these distributions, formulated in the form of various limit theorems. Likewise, in the theory of dynamical systems all the most important notions and problems refer to properties which are asymptotic in time (that is, which take a limit  $t \to \infty$ ). Indeed ergodic theorems, Lyapunov exponents, correlation decay, and limit theorems (CLT, LLT, large deviations, etc) are all time asymptotic properties. In fact all important characteristics and properties of dynamics involve either taking a limit  $t \to \infty$  or averaging over infinite time intervals.

But what happens if a chaotic or stochastic system is in its unique natural (physically observed) stationary state? Such states are described by some (natural) invariant measure on the phase space. These measures, sometimes referred to as "physical" measures, are essentially the only interesting probability distributions on the phase space of a dynamical system or on the space of states of a stochastic system. For example, the uniform measure sitting on a periodic orbit of a chaotic system is invariant but "non-natural".

A general opinion held by both physicists and mathematicians is that nothing interesting happens when the system is in such a stationary state, defined by some invariant measure. Indeed the measure is called invariant because it does not change with time, hence "nothing is changing." At any moment the probability to be in any fixed subset of the phase space is the same as in any other subset having the same measure.

It has been shown, however, that interesting things do happen, at least for the "most" chaotic systems [4]. In fact, transport in the phase space of a dynamical or stochastic system which is in a stationary "physical" state may have interesting and surprising properties. This observation opens the possibility of making finite time predictions about the evolution of chaotic dynamical and stochastic systems.

These studies started with a natural question [4] which seemingly was overlooked in the theory of open dynamical systems [6]. It asks how the escape rate depends on the position of a hole in phase space. This question was inspired by remarkable experiments with atomic billiards [8] where the escape rate of atoms from "billiard tables" was measured. Recall that the escape rate is yet another way to characterize dynamics by taking a limit as time goes to infinity [6].

The escape rate is computed as a limit of a (properly rescaled) survival probability, i.e. of the measure of the set of orbits which have not visited some fixed subset of the phase space (also called a "hole") until a fixed moment in time t. It was proved in [1, 2, 3, 4] that for various classes of dynamical system it is possible to compare survival probabilities (i.e. finite time characteristics of dynamics) for different subsets (different "holes") in the phase

space.

In the present paper we address a much more delicate question which is concerned with first passage (first hitting) probabilities for different subsets of the phase space of chaotic systems or of the state space of stochastic systems. It is a more subtle question because survival probability is an integral (or sum if time is discrete) taken over the interval  $[t, \infty)$  where the integrand is the first passage probability at time s > t. Therefore the first passage probabilities describe transport in the phase space much more precisely than survival probabilities.

Take two subsets A and B of the phase space of some ergodic measure preserving dynamical system and consider the corresponding first passage probabilities  $P_A(t)$  and  $P_B(t)$  for all  $t \ge 0$ . Suppose that  $\mu(A) = \mu(B)$  where  $\mu$  is the corresponding invariant measure. Then it is natural to expect that the curves  $P_A(t)$  and  $P_B(t)$  will intersect infinitely many times (or, perhaps, these curves coincide because of some symmetry of the system under consideration).

Our main result establishes that, quite surprisingly, for a class of the "most" chaotic systems such curves intersect only once after a short interval of time  $[0, t^*]$  where these two curves may initially coincide, unless these curves completely coincide because of some symmetry of dynamics.

The dynamical systems which we consider behave like i.i.d. random variables with stationary uniform distributions on their finite state spaces. Such dynamical systems were called fair dice like systems in [2]. Loosely speaking (see definition in the next section) fair dice like systems are quotients of a full shift with uniform measure. For example the tent map, baker's map, von Neumann-Ulam map, and the Julia sets of rational maps of degree  $d \ge 2$  of the Riemann sphere are all fair dice like systems. Observe that all these systems are discrete time dynamical systems. Therefore the curves of first hitting probabilities are in fact discrete sets. However, the notion of intersection of such "discrete curves" is quite natural. Indeed, if  $P_A(n) \le P_B(n)$  and  $P_A(n + 1) > P_B(n + 1)$  then we say that the

corresponding discrete curves have an intersection on the time interval [n, n + 1].

The subsets A and B that we consider are elements of (possibly different) Markov partitions of the phase space. However, one of these partitions must be a refinement of the other. Still, surprisingly our main result states that there is only a single intersection of the first hitting probability curves for the sets A and B with different measures.

This result allows one to make finite time predictions for chaotic dynamical systems which are in a stationary state. Indeed the entire semi-axis of positive times gets partitioned into three sub-intervals of short, intermediate, and long time. The first two intervals have a finite length while the third one is infinite. By picking a point with a stationary distribution (according to a "physical" invariant measure) we can predict in which element of the initially chosen Markov partition the corresponding orbit will most likely be in at the next moment in the short or long time interval provided that we know the history (itinerary) of this orbit until the present moment of time. In the intermediate interval where (all!) first hitting probability curves intersect each other (unless these curves coincide) the hierarchy of the first hitting probability curves (as functions of time) gets transformed into the opposite hierarchy persisting in the third (long times) interval. Hence finite time predictions about which element of the Markov partition an orbit is more likely to be in first are possible in the interval of short times and in the interval of long times and these predictions are opposite to each other, i.e. the more likely event in the short time interval becomes less likely in the long time interval.

Our results also allow one to find optimal Young towers [9] (in fact optimal bases for towers) such that the tails of recurrence probabilities decay faster than for towers built over other bases. We also prove an estimate of the length of the short time interval which is linear in the length k of symbolic words coding elements of a Markov partition (or its refinements). However, our numerical experiments show that the length of this interval is much longer and grows exponentially in k. The length of the intermediate interval also grows exponentially with the same exponent. It is a strong indication that finite time predictions

for dynamical systems are possible within long time intervals. Moreover, numerical experiments with dispersing billiards [5] demonstrate that this phenomenon (a single intersection of the first hitting probability curves) holds for much larger classes of chaotic dynamical systems for which finite time predictions of the dynamics is therefore also possible.

The structure of the paper is as follows. In the next section we provide necessary definitions and formulate the main results. In section 3 we will introduce some notation and preliminary results. Section 4 contains proofs of the main results for subsets of the phase space with equal measure. Section 5 provides proofs for subsets with different measures. In sections 6 and 7 we prove a linear estimate of the lengths of the time intervals. Numerical results are presented in a short section 8. The last section 9 contains some concluding remarks.

#### 2.2 Definitions and Main Results

Let  $T: M \to M$  be a uniformly hyperbolic dynamical system preserving Borel probability measure  $\mu$ . The following definition [2] singles out a class of dynamical systems analogous to the independent, identically distributed random variables with uniform invariant distributions on their (finite!) state spaces. Classical examples of such stochastic systems are fair coins and dice, hence the corresponding dynamical systems are called fair dice like (FDL) [2].

**Definition 2.2.1.** A uniformly hyperbolic dynamical system preserving Borel probability measure  $\mu$  is called fair dice like or FDL if there exists a finite Markov partition  $\xi$  of its phase space M such that for any integers m and  $j_i$ ,  $1 \le j_i \le q$  one has  $\mu \left( C_{\xi}^{(j_0)} \cap T^{-1} C_{\xi}^{(j_1)} \cap \cdots \cap T^{-m+1} \right)$  $\frac{1}{q^m}$  where q is the number of elements in the partition  $\xi$  and  $C_{\xi}^{(j)}$  is element number j of  $\xi$ .

FDL systems are quotients of a full shift with uniform measure and equal transition probabilities (all equal to  $\frac{1}{a}$ ).

**Example 2.2.1.** Let  $Tx = qx \pmod{1}$  where  $x \in M = [0, 1]$  and  $q \ge 2$  is an integer,

with  $\mu$  the Lebesgue measure. The corresponding Markov partition is the one into equal intervals  $\left[\frac{i}{q}, \frac{i+1}{q}\right], i = 0, 1, \dots, q-1$ .

**Example 2.2.2.** Clearly the tent map with Lebesgue measure is FDL. Consider now the von Neumann-Ulam map of the unit interval into itself. This map T preserves the measure  $\mu$  with density  $\frac{1}{\pi x \sqrt{x(1-x)}}$ . The von Neumann-Ulam map is metrically conjugate to the tent map via the transformation  $y = \sin^2(\frac{\pi x}{2})$ . Therefore it is also FDL.

**Example 2.2.3.** Let  $T : z \to z^2$  be defined on the Riemann sphere. Its Julia set  $\mathcal{J}$  is the unit circle in the complex sphere. Lyubich's measure  $\mu$  that equidistributes periodic points in the Julia set is a continuous probability measure invariant with respect to  $\mu$ . By dividing  $\mathcal{J}$  into  $2^n$  intervals of equal measure we get an FDL system. In fact any rational map defined on the Riemann sphere with degree at least two is an FDL system. By degree here we mean the maximum of the numerator and denominator degree of a rational polynomial.

Let  $\Omega$  denote a finite alphabet of size  $q \ge 2$ . We will call any finite sequence composed of characters from the alphabet  $\Omega$  a string or a word. For convenience both names will be used in what follows without ambiguity. For a fixed string  $w = w_k \dots w_1$ ,  $w_i \in \Omega$  let  $a_w(n)$  denote the number of strings of length n which do not contain w as a substring of consecutive characters. The survival probability for a subset of phase space coded by the string w is then  $\hat{P}_w(n) = \frac{a_w(n)}{q^n}$ .

Denote  $h_w(n) = qa_w(n-1) - a_w(n)$  for  $n \ge k$ . It is easy to see that  $h_w(n)$  equals the number of strings which contain the word w as their last k characters and do not have w as a substring of k consecutive characters in any other place. Therefore  $\frac{h_w(n+k)}{q^{n+k}}$  is the first hitting probability  $P_w(n)$  of the word w at the moment n.

John Conway suggested the notion of autocorrelation of strings (see [10]). Denote by |w| the length of the word w. Let |w| = k. Then the autocorrelation cor(w) of the string w is a binary sequence  $b_k b_{k-1} \dots b_1$  where  $b_i = 1$  if  $w_j = w_{k-i+j}$  for  $j = 1, \dots, i$ , that is, if there is an overlap of size i between the word w and its shift to the right on k-i characters. For example, suppose that w = 10100101. Then cor(w) = 10000101.

Let k = |w|, k' = |w'|, and denote  $h_w(n) = h(n)$  and  $h_{w'}(n) = h'(n)$ . We define

$$s_w = \max_{1 \le j \le k-1} \{ j : b_j = 1 \}$$

whenever this maximum exists and we let s = 0 otherwise. We will always denote  $s = s_w$ and  $s' = s_{w'}$ . In what follows we will generally denote any quantity or function that depends on w' by a superscript '.

Observe that  $\sum_{n=1}^{\infty} P_w(n) = 1 = \sum_{n=1}^{\infty} P_{w'}(n)$ . Clearly if  $P_w(m) - P_{w'}(m) < 0$  for at least one m, there must be at least one n for which  $P_w(n) - P_{w'}(n) > 0$ . Theorem 2 establishes the surprising and fundamental fact that there is only one n for which the quantity  $P_w(n) - P_{w'}(n)$  changes from being negative or zero to positive.

**Theorem 1** Let w and w' be words such that cor(w) > cor(w'). There exists an N > k such that  $h(n) - h'(n) \le 0$  for n < N, and h(n) - h'(n) > 0 for n > N.

Note that  $2^{k-1} \leq cor(w) \leq 2^k - 1$ . Therefore the assumption cor(w) > cor(w') implies  $k \geq k'$ .

One may naturally expect that two discrete curves of survival probabilities intersect infinitely many times unless they coincide. (An obvious example of identical curves provided by two words of the same length where all zeros (ones) in the first word are substituted by ones (zeros)). The next theorem establishes though that nonidentical curves intersect only once.

**Theorem 2** With N as given in Theorem 1 and under the same conditions, there is an N > k such that  $P_w(n) - P_{w'}(n) \le 0$  for n < N, and  $P_w(n) - P_{w'}(n) > 0$  for n > N.

According to Theorems 1 and 2, for two words with different lengths the corresponding

first hitting probabilities curves intersect only at one point. This point divides the positive semi-line into a finite short time interval and an infinite long time interval. Before the moment of intersection it is more likely to hit the smaller subset of phase space (coded by the longer word) for the first time, and after the intersection it is more likely to hit the larger subset for the first time. For two elements of the same Markov partition (which have the same measure) there is also a short initial interval where the two corresponding first hitting probability curves coincide (unless these two curves coincide forever). The length of this initial interval does not exceed the (common) length of the code-words for elements of the Markov partition. After this interval there is a short time interval where it is more likely to visit one element of the Markov partition for the first time, and after this interval there is an infinite, long time interval where it is more likely at any moment to visit the other of these elements for the first time.

Consider now all elements of a Markov partition. They have equal measures because we are dealing with FDL systems. Then there is initial time interval of the length equal the (same) length of words coding elements of this Markov partition. After that comes a finite interval of short times where there is hierarchy of the first hitting probabilities curves. Then comes intermediate interval where (all!) curves intersect. And finally there is infinite interval where there is a hierarchy of the first hitting probabilities curves which is opposite to the one in the short times interval. Therefore finite time predictions of dynamics are possible in the short times interval and in the last infinite long times interval.

The next statement provides an estimate from below of the length of the short time interval.

**Theorem 3** Under the same conditions as Theorem 1 and with N as defined there, if k = k'and s = s' then  $N \ge 4k$ . If k = k' and s > s' then  $N \ge 3k - s$ . If k > k' then N > k + 1.

Let a word w correspond to a subset  $A_w$  of some ergodic dynamical system. Because

 $\mu(A_w) > 0$ , almost all orbits return to the set  $A_w$ . Construct now a Young tower with base  $A_w$ . Denote by  $R_{A_w}(n)$  the probability of first returning to  $A_w$  at the moment n. Let  $P_n(A_w)$  be the first hitting (first passage) probability corresponding to the measure  $\mu$ .

**Definition 2.2.2.** Consider an ergodic dynamical system and choose two subsets A and B of positive measure. We say that tower  $Q_A$  with base A is better than tower  $Q_B$  with base B if there exists  $n^*$  such that  $\sum_{n>n^*} R_A(n) < \sum_{n>n^*} R_B(n)$  for all  $n > n^*$ .

Consider some refinement  $\hat{\xi}$  of the Markov partition  $\xi$ . We say that an element  $C_{\hat{\xi}}$  if the partition  $\hat{\xi}$  is an optimal base for a Young tower out of all elements of  $\hat{\xi}$  if there is no tower better than  $Q_{C_{\hat{\xi}}}$ .

It is well known that

$$P_n(A_w) = \sum_{m > n} R_{A_w}(m)$$

For a given refinement of the Markov partition (as well for the Markov partition itself) it is generally possible to have several optimal bases with equivalent towers built over them. In view of (1) the following statement about an optimal base for a Young tower is an immediate corollary of Theorems 1 and 2.

**Theorem 4** Under the conditions of Theorem 1, for any refinement of a Markov partition  $\xi$  (as well as for the Markov partition itself) there exists an optimal tower with base from this refinement (partition) such that no other of its elements yields a tower better than this one.

A proof of Theorem 1 (see Section 4) implies the following lemma on periodic points and optimal towers. It is well known that for strongly chaotic (hyperbolic) dynamical systems periodic points are everywhere dense. In particular it is true for FDL systems.Denote by  $Per_C$  the minimal period out of all periodic orbits intersecting an element C of some Markov partition. **Lemma 2.2.1.** Let  $\xi$  be a Markov partition of a FDL dynamical system. An element  $C_{\hat{\xi}}$  such that the tower  $Q_{C_{\hat{\xi}}}$  is optimal must have the maximum value of  $Per_C$  out of all other elements of this Markov partition.

Generally an optimal tower for a given Markov partition is not unique, i.e. several elements can serve as optimal bases.

#### 2.3 Results on Pattern Avoidance and Notation

We establish the convention that  $b_0 = 1$  for every word w. The purpose of this convention is to simplify statements like the following, which without this convention do not make sense when (k - s)|k, for example. By the definition of cor(w)

if 
$$b_j = 1$$
 for some  $j \in \{0, 1, \dots, k-1\}$ ,  
then  $b_{k-(k-j)t=1}$  for all  $t \in \{1, \dots, \lfloor \frac{k}{k-j} \rfloor\}$ , (2.1)

(see ([11])).

Given *i* such that  $b_i = 1$ , let  $[i] = \max \{j : b_j = 1 \text{ and } i = k - t(k - j) \text{ for some } 1 \le t \le \lfloor \frac{k}{k-j} \rfloor\}$ . In light of the relation (2.1), it is natural to define the set  $I = \{[i] : b_i = 1\}$ .

We will need to distinguish a few digits of the autocorrelation in addition to s. Let

$$d = \min_{j \in I} \{ j : b_j = 1 \}$$
  

$$r = \max_{j \in I} \{ j : b_j = 1 \text{ and } b'_j = 0 \}$$

whenever they exist.

The largest member of I is always s. An effect of Propositions 2.4.1 and 2.4.2 below is that  $I \subset \{1, ..., k - s - 2\} \cup \{s\}$ . A further consequence of Proposition 2.4.1 is that the only member i of I for which  $|\{j : [j] = i\}| > 1$  is s, hence we define  $S = \{i : [i] = s\}$ .

Let  $H_w(n)$  be the number of strings which end with w, begin with w, and which do not

contain w as a substring of k consecutive characters in any other place. For n > k it is easy to see that H(n) = qh(n-1) - h(n). The probability of first returning to the "hole" given by w is  $\frac{H_w(n)}{q^n}$ .

While  $H_w(n) > 0$  for n > 2k,  $H_w(2k) = 0$  if and only if there is an *i* for which  $b_i = b_{k-i} = 1$ . It is easy to see that the condition  $b_i = b_{k-i} = 1$  implies  $b_{k-s} = 1$ , and this in turn can be used to prove that (k - s)|k. We can thus evaluate  $H_w(n)$  for  $n \le 2k$  as follows.

$$H_w(n) = \begin{cases} 0 & \text{if } n < k, \\ -1 & \text{if } n = k, \\ 1 & \text{if } n = 2k - i \text{ for some } i \in I, \\ 0 & \text{otherwise if } n < 2k \\ 0 & \text{if } n = 2k \text{ and } (k - s) | k \\ 1 & \text{if } n = 2k \text{ and } (k - s) \nmid k. \end{cases}$$
(2.2)

It was proved in [11] that

$$h_w(n) \ge \begin{cases} (q-1)\sum_{t=1}^{k-s} h_w(n-t) & \text{if } 0 < s < k, \\ (q-1)\sum_{t=1}^{k-1} h_w(n-1) & \text{if } s = 0, \end{cases}$$
(2.3)

and

$$h_w(n) = qh_w(n-1) - h_w(n-k) + \sum_{t=1}^{k-1} b_t H_w(n-k+t).$$
(2.4)

The latter formula is derived from the following relation [10].

$$h_w(n) = \sum_{t=1}^k b_i H_w(n+t).$$
 (2.5)

It is easy to see that  $H(n) \leq h(n-k)$  for n > k, and we will prove below that  $(q-1)h(n-k-1) \leq H(n)$  for n > k+1. This result is the content of Corollary 2.4.2.

#### 2.4 A Proof of Theorems 1 and 2 when k and k' are equal

We prove in this section several technical results which will be used to deduce Theorems 1-2. We remark that Theorem 2 is equivalent to the claim that an N > k exists such that  $h(n) - q^{k-k'}h'(n-k+k') \le 0$  for n < N and  $h(n) - q^{k-k'}h'(n-k+k') > 0$  for  $n \ge N$ .

For any  $i \in I$  let  $T_w(i) = \max\{t > 0 : w_{k-i} \dots w_{k-i-t+1} = w_{k-j} \dots w_{k-j-t+1}$  for some  $j \in I, j > i\}$ , with the convention that if the latter set is empty then  $T_w(i) = 0$ . Again we will often denote  $T(i) = T_w(i)$  when w is fixed.

**Proposition 2.4.1.** *Let*  $i \in I - \{s\}$ *. Then* i + T(i) < k - s*.* 

*Proof.* For any *i* such that  $b_i = 1$  and for any *t* satisfying  $k - i \leq t \leq k$  one has  $w_t \dots w_{t-(k-i)+1} = w_{t-l(k-i)} \dots w_{t-(l+1)(k-i)+1}$  for  $0 \leq l \leq \lfloor \frac{t}{k-i} \rfloor - 1$ . Further, if  $e = t - \lfloor \frac{t}{k-i} \rfloor (k-i)$  and e > 0 then  $w_t \dots w_{t-e+1} = w_e \dots w_1$ . This is a consequence of the structure of the correlation function as described by (2.1). Therefore when  $b_i = 1$  we will say that *w* contains a k - i period.

Let  $i \in I$ . Suppose first that T(i) > 0 and for a contradiction suppose that  $i + T(i) \ge k - s$ . Let  $i' \in I$ , i' > i be such that  $w_{k-i} \dots w_{k-i-T(i)+1} = w_{k-i'} \dots w_{k-i'-T(i)+1}$ .

Since  $b_{i'} = 1, w_{i'} \dots w_1 = w_k \dots w_{k-i'+1}$  which implies  $w_{k-(i'-i)} \dots w_{k-i'+1} = w_{i'-(i'-i)} \dots w_1 = w_k \dots w_{k-i+1}$ . Since  $b_i = 1$ , similarly one has

$$w_{k-(i'-i)}\dots w_{k-i'+1} = w_k\dots w_{k-i+1}.$$
 (2.6)

Since  $i - (k - s) \ge -T(i)$  we have  $w_{k-i'} \dots w_{k-i'+i-(k-s)+1} = w_{k-i} \dots w_{k-i+i-(k-s)+1} = w_{k-i} \dots w_{s+1}$ . Therefore

$$w_{k-(i'-i)} \dots w_{k-(i'-i)-(k-s)+1} = w_k \dots w_{k-i+1} w_{k-i'} \dots w_{k-(i'-i)-(k-s)+1}$$
$$= w_k \dots w_{k-i+1} w_{k-i} \dots w_{s+1} = w_k \dots w_{s+1},$$

where we have used (2.6) in the first equality.

Since w contains a k - s period,

$$w_{k-(i'-i)-l(k-s)} \dots w_{k-(i'-i)-(l+1)(k-s)+1}$$
  
=  $w_{k-(i'-i)} \dots w_{k-(i'-i)-(k-s)+1} = w_k \dots w_{s+1}$   
=  $w_{k-l(k-s)} \dots w_{k-(l+1)(k-s)+1}$  (2.7)

for every  $0 \le l \le \lfloor \frac{k-i}{k-s} \rfloor - 1$ . Further, for  $e = k - (i'-i) - \lfloor \frac{k-(i'-i)}{k-s} \rfloor (k-s)$ , if e > 0 one has

$$w_{e} \dots w_{1} = w_{k-(i'-i)} \dots w_{k-(i'-i)-e+1}$$

$$= w_{k-\lfloor \frac{k-(i'-i)}{k-s} \rfloor (k-s)} \dots w_{i'-i+1}$$
(2.8)

Together, 2.7 and 2.8 imply that  $w_{k-(i'-i)} \dots w_1 = w_k \dots w_{i'-i+1}$ , or that  $b_{k-(i'-i)} = 1$ .

Our goal now is to show that there is some index  $i^*$  such that  $b_{i^*} = 1$ ,  $i^* > i$ , and  $i = k - l(k - i^*)$  for some l > 0. Doing this would contradict the fact that  $i \in I$ . Let  $d_0 = i' - i$ . We will construct a strictly decreasing sequence  $\{d_n\}_{n=0}^N$  of positive integers

such that  $b_{k-d_n} = 1$ ,  $d_n = k - l_n d_{n-1} - i$  where  $l_n$  is the unique positive integer such that  $k - l_n d_{n-1} > i > k - (l_n + 1)d_{n-1}$ , and  $i^* = k - d_N$  has the desired property.

If there is some t for which  $k - td_0 = i'$  then  $k - (t + 1)d_0 = i$ , and we may take N = 0. Similarly N = 0 if  $k - td_0 = i$  for some t. Otherwise, there exists t for which  $i' > k - td_0 > i$ . Since  $b_{k-d_0} = 1$ , the word w contains a  $d_0$  period. With  $d_1 = k - td_0 - i$  it is easy to see that  $b_{k-d_1} = 1$  (a more detailed exposition for general n is below).

For n > 1 suppose that  $d_{n-1}$  is already defined. If  $i \neq k - ld_{n-1}$  for some l > 0then N = n - 1. In addition one cannot have  $k - l_n d_{n-1} = k - l_{n-1} d_{n-2}$  as this implies  $i - (k - l_n d_{n-1}) = i - (k - l_{n-1} d_{n-2}) = d_{n-1}$  hence  $k - (l_n - 1)d_{n-1} = i$ , and again N = n - 1. Otherwise denote  $\iota = k - l_{n-1}d_{n-2}$  and observe that there is some  $l_n$  such that  $\iota > k - l_n d_{n-1} > i$ . Since w contains a  $d_{n-1}$  period, we will show that  $b_{k-l_n d_{n-1}-i} =$  $b_{k-d_n} = 1$ . Let  $\delta = \iota - (k - l_n d_{n-1})$ . Observe that with this notation,  $d_{n-1} = \delta + d_n$ .

For any  $0 \le l < \lfloor \frac{k-d_n}{d_{n-1}} \rfloor$  one has

$$w_{k-d_n-ld_{n-1}} \dots w_{k-d_n-(l+1)d_{n-1}+1} = w_{k-d_n-(l_n-1)d_{n-1}} \dots w_{k-d_n-l_nd_{n-1}+1}$$
$$= w_{\iota} \dots w_{i+1}$$
$$= w_k \dots w_{k-d_{n-1}}$$
$$= w_{k-ld_{n-1}} \dots w_{k-(l+1)d_{n-1}}.$$

In the first equality we have used the  $d_{n-1}$  periodicity of w, in the second we have used the fact that  $k - d_n - (l_n - 1)d_{n-1} = \iota$ , in the third that  $b_{\iota} = 1$ , and again in the fourth the  $d_{n-1}$  periodicity of w.

Let 
$$e = k - d_n - \lfloor \frac{k - d_n}{d_{n-1}} \rfloor d_{n-1}$$
. If  $e > 0$  and  $e < \delta$  then one has

$$w_e \dots w_1 = w_{k-l_n d_{n-1} - d_n} \dots w_{k-l_n d_{n-1} - d_n - e+1}$$
$$= w_i \dots w_{i-e+1}$$
$$= w_k \dots w_{k-e+1}$$

$$= w_{k-\lfloor \frac{k-d_n}{d_{n-1}} \rfloor d_{n-1}} \dots w_{d_n+1}.$$

If e > 0 and  $e > \delta$  then

$$w_e \dots w_1 = w_i \dots w_{i-\delta+1} w_{i-\delta} \dots w_{i-e+1}$$
$$= w_k \dots w_{k-\delta+1} w_{k-\delta} \dots w_{k-e+1}$$
$$= w_k \dots w_{k-e+1}$$
$$= w_{k-\lfloor \frac{k-d_n}{d_{n-1}} \rfloor d_{n-1}} \dots w_{d_n+1}.$$

One thus has  $w_{k-d_n} \dots w_1 = w_k \dots w_{d_n+1}$  and  $b_{k-d_n} = 1$ . Since  $d_n < d_{n-1}$  as long as  $[i] \neq k - d_{n-1}$ , the sequence  $\{d_n\}$  is strictly decreasing. Since  $k - d_n$  is bounded below by 1, there must be some n for which  $[i] = k - d_n$ , and we let N = n.

If T(i) = 0, the proof is similar to what we have just done. Supposing i + T(i) = i > k - s, there is some t for which k - t(k - s) > i > k - (t + 1)(k - s), otherwise [i] = s and  $i \notin I$ . Since w contains a k - s period, one can show that  $b_{k-t(k-s)-i} = 1$ . Again we can construct a strictly increasing sequence of integers  $\{i_n\}_{n=0}^N$  such that  $b_{i_n} = 1$  and  $[i] = i_N$ . We omit the proof due to its redundancy.

**Corollary 2.4.1.**  $\{i : b_i = 1\} = \{i : [i] = s\} \cup (I - \{s\}).$ 

*Proof.* For  $i \in I - \{s\}$  one has i < s and i < k - s, hence  $i < \frac{k}{2}$ . If  $b_j = 1$  and  $j \neq k - t(k - s)$  for any t, then j = k - l(k - i) for some  $i \in I - \{s\}$  if and only if l = 1 since  $k - i > \frac{k}{2}$ . Thus either  $j \in \{i : [i] = s\}$  or j = i for some  $i \in I - \{s\}$ .

**Corollary 2.4.2.**  $H(n) \ge (q-1)h(n-k-1)$  for n > k+1.

*Proof.* Observe that (2.2) implies  $H(n) \ge 0 = (q-1)h(n-k-1)$  for  $k+1 < n \le 2k$ .

Let 2k < n < 3k - s. For  $1 \le i \le s$  one has  $k + i < n - k + i < 2k - s + i \le 2k$ , so by (2.2) we have H(n - k + i) = 1 if and only if  $b_{3k-n-i} = 1$  and  $3k - n - i \in I$ . If  $3k - n - i \in I - \{s\}$  then 3k - n - i < k - s by Proposition 1 and hence  $b_{3k-n-i} = 0$ for  $n \leq 2k + s - i$ . In particular,  $b_{3k-n-i} = 0$  when n = 2k + 1 and  $i \in I - \{s\}$ . Thus  $\sum_{i=1}^{s} b_i H(k - i + 1) \leq 1$  and  $\sum_{i=1}^{s} b_i H(n - k + i) \leq n - 2k$ . Since  $h(n) = q^{n-k}$  for  $k \leq n < k - s$  one has

$$\begin{split} H(n) &= h(n-k) - \sum_{i=1}^{s} b_i H(n-k+i) \\ &= q q^{n-2k-1} - \sum_{i=1}^{s} b_i H(n-k+i) \\ &= (q-1)q^{n-2k-1} + \left(q^{n-2k-1} - \sum_{i=1}^{s} b_i H(n-k+i)\right) \\ &\geq (q-1)q^{n-2k-1} + \left(q^{n-2k-1} - (n-2k)\right) \\ &\geq (q-1)q^{n-2k-1} = (q-1)h(n-k-1). \end{split}$$

For  $n \ge 3k - s$  observe that  $\sum_{i \in S} H(n - k + i) \le \sum_{i=1}^{k} b_i H(n - 2k + s + i) = h(n - 2k + s)$ . Then one has

$$\begin{split} H(n) &= h(n-k) - \sum_{i=1}^{s} b_i H(n-k+i) \\ &= h(n-k) - \sum_{i \in S} H(n-k+i) - \sum_{i \in I - \{s\}} H(n-k+i) \\ &\geq h(n-k) - h(n-2k+s) - \sum_{i \in I - \{s\}} h(n-2k+i) \\ &\geq (q-1) \sum_{t=1}^{k-s} h(n-k-t) - h(n-2k+s) - \sum_{i=1}^{k-s-2} h(n-2k+s+i) \\ &\geq (q-1)h(n-k-1) \end{split}$$

where we have used Corollary 2.4.1.

**Proposition 2.4.2.** Suppose that  $s \neq k-1$ . Then either  $b_{t(k-s)} = 0$  for every  $1 \leq t \leq \lfloor \frac{k}{k-s} \rfloor$ or  $b_{t(k-s)-1} = 0$  for every  $1 \leq t \leq \lfloor \frac{k+1}{k-s} \rfloor$ 

*Proof.* We use the following two statements, the first of which is obvious from Proposition 1.

If 
$$b_{k-s} = 1$$
 then  $[k-s] = s$ . (2.9)

If 
$$b_{k-s-1} = 1$$
 then  $[k-s-1] = s$ . (2.10)

We prove (2.10). Suppose  $b_{k-s-1} = 1$ . If  $b_{k-s} = 1$  then  $b_t = 1$  for every  $1 \le t \le k-s$  and so  $w_t = w_k$  for every  $1 \le t \le k-s$ . Since w contains a k-s period  $w = \underbrace{w_k * \cdots * w_k}_{k \text{ times}}$ and [k-s-1] = s.

If  $b_{k-s} = 0$  then either k - s - 1 = s and the result follows, or there is some t > 0such that k - t(k - s) > k - s. Let i = k - s - 1,  $\iota = k - t(k - s)$ , and  $d = \iota - i$ . Since  $b_{\iota} = 1$  and  $b_i = 1$  it is easy to see that  $w_{\iota} \dots w_1$  contains a d period. As a result  $b_{\iota-ld} = 1$  for every  $1 \le l \le \lfloor \frac{\iota}{d} \rfloor$ . Let L be such that  $\iota - Ld > k - (k+1)(k-s) > 0$  and  $\iota - (L+1)d \le k - (k+1)(k-s)$ . If  $d \nmid (k-s)$  then  $\iota - Ld - (k - (k+1)(k-s)) = d' < d$ . Since  $b_{\iota-Ld} = 1$  and  $b_{k-(k+1)(k-s)} = 1$  it must be that  $w_{\iota} \dots w_1$  contains a d' period, and hence  $b_{\iota-d'} = 1$ . Since  $\iota - d' > \iota - d = k - s - 1$ , with  $i' = [\iota - d']$  one has  $[i'] \ne s$ and  $[i'] + T([i']) \ge k - s$ , a contradiction to Proposition 1. It follows that d|(k - s) which implies that w itself contains a d period. Then  $b_{k-d} = 1$  but since d < k - s this contradicts the definition of s.

The following statement is a corollary of (2.9) and (2.10).

Suppose that 
$$s \neq k-1$$
. Then  $I - \{s\} \subset \{1, \dots, k-s-2\}$ .

If  $b_{t(k-s)} = 1$  for some t > 1 then by Proposition (2.4.1) it must be that [t(k-s)] = sand hence there is some l such that k - l(k-s) = t(k-s), whence (k-s)|k. According to (2.1) it must be that  $b_{k-s} = 1$  as well. Thus, if  $b_{k-s} = 0$  then  $b_{t(k-s)} = 0$  for every t. If  $b_{k-s} = 1$  then  $b_{k-s-1} = 0$  as otherwise s = k-1. If  $b_{t(k-s)-1} = 1$  for some t > 1 then [t(k-s)-1] = s and k = m(k-s) - 1. Since  $b_{k-t(k-s)} = 1$ , one has  $b_{(m-t)(k-s)-1} = 1$ for every  $1 \le t \le m-1$ . With t = m-1 this implies in particular that  $b_{k-s-1} = 1$ , a contradiction. Thus  $b_{t(k-s)-1} = 0$  for every t > 1.

**Lemma 2.4.1.** If s > 0,  $1 \le l \le k-1$ , and  $n \ge 2k+l$  then  $H(n) \ge (q-1)\sum_{t=1}^{l} H(n-t)$ .

*Proof.* Rearranging relation (2.5) we obtain

$$H(n) = h(n-k) - \sum_{t=1}^{k-1} b_t H(n-k+t) = h(n-k) - \sum_{i=1}^{s} b_i H(n-k+i).$$
(2.11)

Using (2.11) one has

$$H(n) - (q-1) \sum_{t=1}^{l} H(n-t) = h(n-k) - (q-1) \sum_{t=1}^{l} h(n-k-t)$$
  

$$- \sum_{i=1}^{s} b_i H(n-k+i) + (q-1) \sum_{t=1}^{l} \sum_{i=1}^{s} b_i H(n-k+i-t) =$$
  

$$h(n-k-l) - \sum_{t=0}^{l-1} H(n-k-t)$$
  

$$- \sum_{i=1}^{s} b_i \left( H(n-k+i) - (q-1) \sum_{t=1}^{l} H(n-k+i-t) \right).$$
  
(2.12)

For any  $i \in I - \{d\}$  let  $\tilde{i} = \max \{\iota < i : b_{\iota} = 1\}$ . Observe that  $|i - \tilde{i}| \leq k - s$  since  $b_{k-t(k-s)} = 1$  always. It follows that  $\tilde{i} = i - \tau$  for some  $1 \leq \tau \leq k - s$ . We have

$$\sum_{i=1}^{s} b_{i} \left( H(n-k+i) - (q-1) \sum_{t=1}^{l} H(n-k+i-t) \right) \leq \sum_{i \in I - \{d\}} \left( H(n-k+i) - H(n-k+\tilde{i}) \right) + H(n-k+d) - (q-1) \sum_{t=1}^{l} H(n-k+d-t) \leq H(n-l) - \sum_{t=0}^{l-1} H(n-k-t).$$

$$(2.13)$$

where we have used the fact that  $n \ge 2k + l$  to ensure that n - k + i - t > k for every i, hence H(n - k + i - t) > H(k) = -1. Combining (2.13) and (2.12) one has

$$H(n) - (q-1) \sum_{t=1}^{l} H(n-t) \ge$$

$$h(n-k-l) - \sum_{t=0}^{l-1} H(n-k-t) - H(n-l) + \sum_{t=0}^{l-1} H(n-k-t) \ge$$

$$h(n-k-l) - H(n-l) \ge 0.$$
(2.14)

Let 
$$\Delta(n) = h(n) - h'(n)$$
.

**Corollary 2.4.3.** Suppose w' is such that  $cor(w) \ge cor(w')$ , k = k', and  $n \ge 3k$ . If  $\Delta(n-t) \ge (q-1)\Delta(n-t-1)$  for  $1 \le t \le k-1$  then  $\Delta(n) \ge (q-1)\Delta(n-1)$ .

*Proof.* There are three cases. In the first 1 < r < k - 1, in the second r = k - 1, and in the third r = 1. In the first case, using (2.4) one has

$$\Delta(n) = q\Delta(n-1) - \Delta(n-k) + \sum_{i=r+1}^{k-1} b_i [q\Delta(n-k+i-1) - \Delta(n-k+i)] + \sum_{i=1}^r b_i H(n-k+i) - \sum_{i=1}^{r-1} b'_i H'(n-k+i)$$
(2.15)

Using the equality  $H(n)-H'(n)=q\Delta(n-1)-\Delta(n)$  and applying Lemma 1 one has

$$\sum_{i=1}^{r} b_i H(n-k+i) - \sum_{i=1}^{r-1} b'_i H'(n-k+i)$$
  

$$\geq \sum_{i=1}^{r-1} H(n-k+i) - \sum_{i=1}^{r-1} H'(n-k+i)$$
  

$$= \sum_{i=1}^{r-1} q\Delta(n-k+i-1) - \Delta(n-k+i)$$

The expression (2.15) is thus bounded below by

$$q\Delta(n-1) - \Delta(n-k) + \sum_{i=r+1}^{k-1} b_i [q\Delta(n-k+i-1) - \Delta(n-k+i)] + \sum_{i=1}^{r-1} [q\Delta(n-k+i-1) - \Delta(n-k+i)].$$

By using the inductive assumption it is easy to see that  $\Delta(n-1) + \sum_{i=r+1}^{k-1} b_i [g\Delta(n-k+i-1) - \Delta(n-k+i)] \ge (q-1)\Delta(n-k+r)$  and  $\Delta(n-k+r) + \sum_{i=1}^{r-1} [q\Delta(n-k+i-1) - \Delta(n-k+i)] \ge (q-1)\Delta(n-k)$ . (For a more detailed explanation, see [11]). Applying both bounds, we have  $\Delta(n) \ge (q-1)\Delta(n-1) - \Delta(n-k) + (q-1)\Delta(n-k) \ge (q-1)\Delta(n-1)$ .

Suppose now that r = k - 1, hence s = r = k - 1 and  $b_i = 1 \forall i$ . We have

$$\Delta(n) = q\Delta(n-1) - \Delta(n-k) + H(n-1) + \sum_{t=1}^{k-2} H(n-k-i) - b'_i H'(n-k-i)$$
  

$$\geq q\Delta(n-1) - \Delta(n-k) + H(n-1) + \sum_{t=1}^{k-2} [q\Delta(n-k+i-1) - \Delta(n-k+i)].$$
(2.16)

Noting that H(n-1) > 0 since  $n \ge 3k$ , by subtracting H'(n-1) from (2.16) we obtain

$$\Delta(n) \ge (q-1)\Delta(n-1) - \Delta(n-k)$$
$$+ \Delta(n-1) + \sum_{t=1}^{k-2} [q\Delta(n-k+t-1) - \Delta(n-k+t)]$$

Using  $\Delta(n-1) > \Delta(n-2)$  as before we have that

$$\Delta(n) > (q-1)\Delta(n-1) - \Delta(n-k) + (q-1)\Delta(n-k)$$
  
 
$$\geq (q-1)\Delta(n-1).$$

Finally suppose that r = 1. Then

$$\begin{aligned} \Delta(n) &= q\Delta(n-1) - \Delta(n-k) + \sum_{t=2}^{k=1} b_t [q\Delta(n-k+t-1) - \Delta(n-k+t)] + H(n-k+1) \\ &\geq (q-1)\Delta(n-1) - \Delta(n-k) + (q-1)\Delta(n-k+1) \\ &\geq (q-1)\Delta(n-1). \end{aligned}$$

Corollary 2.4.4. Let  $n \ge 4k$ . Then  $\sum_{t=0}^{k-d-1} H(n-k-t) \ge \sum_{i \in I} \sum_{t=1}^{k-i} b_t H(n-2k+i+t)$ Proof. For  $i \in I - \{s\}$ , applying Lemma 1 we have

$$\sum_{t=1}^{k-i} b_t H(n-2k+i+t) = \sum_{t=1}^{s} b_t H(n-2k+i+t)$$
  
$$\leq H(n-2k+i+s+1).$$

Note that  $I - \{s\} \subset \{1, \dots, k - s - 2\}$ . If  $b_{k-s-2} = 1$  and  $b_{k-s} = 1$  or  $b_{k-s-1} = 1$  then  $I = \{s\}$  and the statement of the lemma holds. It suffices to assume that either  $b_{k-s-2} = 0$  or  $b_{k-s} = b_{k-s-1} = 0$ .

If  $b_{k-s-2} = 0$  then  $s \neq k-1$  and for  $i \in I$  one has  $i+s+1 \leq k-s-2$ . Since it always true that one of  $b_{k-s}$  or  $b_{k-s-1} = 0$  when  $s \neq k-1$  (see Proposition 2) one must have

$$-H(n-k) - H(n-k-1) + \sum_{t=1}^{k-s} b_t H(n-2k+s+t) \le 0$$

Since  $i + s + 1 \le k - s - 2$  for  $i \in I - \{s\}$  we thus have

$$-\sum_{t=0}^{k-d-1} H(n-k-t) + \sum_{i \in I} \sum_{t=1}^{k-i} b_t H(n-2k+i+t)$$
  
$$\leq -H(n-k) - H(n-k-1) + \sum_{t=1}^{k-s} b_t H(n-2k+s+t)$$

 $\leq 0.$ 

If both  $b_{k-s} = 0$  and  $b_{k-s-1} = 0$  then

$$-H(n-k) + \sum_{t=1}^{k-s} b_t H(n-2k+s+t) \le 0.$$

For  $i \in I$  one has  $i + s + 1 \le k - s - 1$  and

$$-\sum_{t=0}^{k-d-1} H(n-k-t) + \sum_{i\in I} \sum_{t=1}^{k-i} b_t H(n-2k+i+t)$$
  
$$\leq -H(n-k) + \sum_{t=1}^{k-s} b_t H(n-2k+s+t)$$
  
$$\leq 0.$$

**Corollary 2.4.5.** Let n > 2k. Then  $H(n) \ge \sum_{i \in I} H(n - k + i)$ .

*Proof.* Let 2k < n < 3k - s. For  $i \neq s$  observe that n - k + i < n - 2k + s < k, hence H(n - k + i) = 0. It follows that

$$H(n) - \sum_{i \in I} H(n - k + i) = H(n) - H(n - k + s) \ge H(n) - 1 \ge 0.$$

Note that  $|I| \le k - s$  and recall  $s \le k - 1$ . For  $n \ge 3k - s$  one has

$$H(n) - \sum_{i \in I} H(n - k + i) \ge H(n) - \sum_{i=1}^{k-s} H(n - i) \ge 0$$

by application of Lemma 1.

**Corollary 2.4.6.** Let  $n \ge 2k$ . Then  $h(n) \ge \sum_{t=1}^{k-1} H(n+t)$ .

Proof. Applying Lemma 1, one has

$$h(n) = \sum_{t=1}^{k} b_t H(n+t) \ge \sum_{t \in S \cup \{k\}} H(n+t) \ge \sum_{t=1}^{k-1} H(n+t).$$

Let  $S = \{\iota : [\iota] = s\}$ . If  $\iota \in S - \{s\}$  then

$$h(n-2k+\iota) - \sum_{j=1}^{s} b_j H(n-2k+\iota+j) - H(n-2k+s+\iota+(k-s)) = 0.$$

It follows that

$$\sum_{\iota \in S-\{s\}} \left( h(n-2k+\iota) - \sum_{j=1}^{s} b_j H(n-2k+\iota+j) \right) \\ + h(n-2k+s) - \sum_{j=1}^{s} b_j H(n-2k+s+j) \\ = \sum_{\iota \in S-\{s\}} \left( h(n-2k+\iota) - \sum_{j=1}^{s} b_j H(n-2k+\iota+j) - H(n-2k+s+\iota+(k-s)) \right) \\ + h(n-2k+s) - \sum_{j=1}^{k-s} b_j H(n-2k+s+j).$$

From this one has

$$\sum_{\iota=1}^{k-1} b_i H(n-k+\iota) = \sum_{\iota\in S} H(n-k+\iota) + \sum_{\iota\in I-\{s\}} H(n-k+\iota) = \sum_{\iota\in S} \left( h(n-2k+\iota) - \sum_{t=1}^{k-1} b_t H(n-2k+\iota+t) \right) + \sum_{\iota\in I-\{s\}} \left( h(n-2k+\iota) - \sum_{t=1}^{k-1} b_t H(n-2k+\iota+t) \right) =$$

$$h(n-2k+s) - \sum_{t=1}^{k-s} H(n-2k+s+t) + \sum_{\iota\in I-\{s\}} \left( h(n-2k+\iota) - \sum_{t=1}^{k-\iota} b_t H(n-2k+\iota+t) \right).$$
(2.17)

**Lemma 2.4.2.** If k = k' and  $s \neq s'$  then  $\Delta(n) \leq 0$  for n < 3k - s. If s = s' then  $\Delta(n) \leq 0$  for n < 4k.

The proof of Lemma 2.4.2 when s = s' is divided into two parts which constitute sections 6 and 7 below. We include the proof when  $s \neq s'$  here.

*Proof.* We remark that  $\Delta(n) \leq 0$  for  $n \leq 2k$  and  $\Delta(n) = 0$  for n < 2k - r no matter the values of s and s'.

Using (2.11) one has

$$H(n) - H'(n) = \Delta(n-k) - \sum_{i=1}^{s} b_i H(n-k+i) - b'_i H'(n-k+i).$$
(2.18)

Suppose that r = s. There are two cases;  $b_t - b'_t = -1$  for  $1 \le t \le s - 1$ , or  $b_\tau - b'_\tau = 0$  for some  $\tau < s$ . In the first case note that s' = s - 1, and observe that one must have  $s \le k - s$ . Otherwise  $s > s - (k - s) \ge 1$  and since s - (k - s) = k - 2(k - s) one has  $b_{k-2(k-s)} - b'_{k-2(k-s)} \ge 0$ , a contradiction.

From (2.18) for n < 3k - s one has

$$H(n) - H'(n) = -H(n-k+s) + \sum_{t=1}^{s-1} H'(n-k+t) \ge -H(n-k+s).$$

It is thus easy to see that

$$H(n) - H'(n) \ge \begin{cases} 0 & 2k < n < 3k - 2s \\ -1 & 3k - 2s \le n < 3k - s. \end{cases}$$

Since  $\Delta(2k) \leq -1$ , using the relation

$$\Delta(n) = q\Delta(n-1) - H(n) + H'(n)$$

one has

$$\Delta(n) \le \begin{cases} q\Delta(n-1) & 2k < n < 3k - 2s \\ q\Delta(n-1) + 1 & 3k - 2s \le n < 3k - s. \end{cases}$$

It follows that  $\Delta(n) \leq 0$  for n < 3k - s.

We now suppose that  $b_{\tau} - b_{\tau}' = 0$  for some  $1 < \tau < s$ . One has

$$\Delta(2k) \le -q^s + \sum_{t=1}^s q^{s-t} - q^{s-\tau} \le -2.$$
(2.19)

From (2.18) one has

$$H(n) - H'(n) \ge -\sum_{i=1}^{s} b_i H(n-k+i),$$

from which we obtain the upper bound

$$H(n) - H'(n) \ge -(n - 2k).$$

It follows that

$$\Delta(n) \le q\Delta(n-1) + (n-2k). \tag{2.20}$$

The inequality (2.20) together with (2.19) implies

$$\Delta(n) \le -2 - (n - 2k) \text{ for } 2k < n < 3k - s$$

and the result follows.

**Lemma 2.4.3.** Let k = k' and  $N \ge 4k$ . Suppose h(N) > h'(N) and that  $h(n) \le h'(n)$  for n < N. Then  $H(n) - H'(n) \le 0$  for  $N \le n \le N + k$ ; In particular  $\Delta(n) > (q-1)\Delta(n-1)$  for  $N \le n \le N + k$ .

*Proof.* Suppose that r = s, and observe that this is equivalent to the condition s > s'. By Lemma 4.2 we may assume that  $N \ge 3k - s$ . From (2.11), (2.17), and (2.22) one has

$$\begin{split} H(n) &\leq h(n-k) - \sum_{i \in S} H(n-k+i) \\ &= h(n-k) - h(n-2k+s) + \sum_{t=1}^{k-s} b_t H(n-2k+s+t) \\ &= (q-1) \sum_{t=1}^{k-s} h(n-k-t) - \sum_{t=0}^{k-s-1} H(n-k-t) + \sum_{t=1}^{k-s} b_t H(n-2k+s+t) \\ &\leq (q-1) \sum_{t=1}^{k-s} h(n-k-t). \end{split}$$

To summarize,

$$H(n) \le (q-1) \sum_{t=1}^{k-s} h(n-k-t).$$
(2.21)

For any L > 0 one has

$$h(n) = (q-1)\sum_{t=1}^{L} h(n-t) - \sum_{t=0}^{L-1} H(n-t).$$
(2.22)

Note that s' < k-1. From Proposition 2.4.2 there exists  $\iota \in \{0, 1\}$  such that  $b'_{t(k-s')-\iota} = 0$  for every  $1 \le t \le U$  where  $U = \lfloor \frac{k+\iota}{k-s'} \rfloor$ . Using (2.3) and (2.22) one has

$$\begin{split} H'(n) &\geq h'(n-k) - \sum_{i=1}^{s'} b'_i h'(n-2k+i) \\ &= (q-1) \sum_{t=1}^k h'(n-k-t) - \sum_{t=0}^{k-1} H'(n-k-t) - \sum_{i=1}^{s'} b'_i h'(n-2k+i) \\ &\geq (q-1) \sum_{t=1}^{k-s'-1} h'(n-k-t) - \sum_{t=0}^{k-1} H'(n-k-t) \\ &+ \sum_{t=1}^U h'(n-2k-\iota+t(k-s')) + h'(n-2k) \\ &= (q-1) \sum_{t=1}^{k-s'-1} h'(n-k-t) + \left( h'(n-2k) - \sum_{l=1}^{k-s'-\iota} H'(n-2k+l) \right) \\ &+ \sum_{t=1}^{U-1} \left( h'(n-2k-\iota+t(k-s')) - \sum_{l=1}^{k-s'} H'(n-2k-\iota+t(k-s')+l) \right) \\ &+ \left( h'(n-2k-\iota+U(k-s')) - \sum_{l=1}^{k+\iota-U(k-s')} H'(n-2k-\iota+U(k-s')+l) \right) \\ &\geq (q-1) \sum_{t=1}^{k-s'-1} h'(n-k-t). \end{split}$$

Thus

$$H'(n) \ge (q-1) \sum_{t=1}^{k-s'-1} h'(n-k-t).$$
(2.23)

Using (2.21) and (2.23) it follows that

$$H(n) - H'(n) \le (q-1)\sum_{t=1}^{k-s} h(n-k-t) - (q-1)\sum_{t=1}^{k-s'-1} h'(n-k-t) \le 0$$

for  $N \leq n < N + k$ .

Suppose that  $r \neq s$ , equivalently s = s'. By Lemma 2.4.2 we may assume that  $n \geq 4k$ . By use of Corollary 2.4.4 and equality (2.17) one has

$$\begin{split} H(n) &= h(n-k) - \sum_{i \in I} h(n-2k+i) + \sum_{i \in I} \sum_{t=1}^{s} b_t H(n-2k+i+t) \\ &= (q-1) \sum_{t=1}^{k-d} h(n-k-t) - \sum_{t=0}^{k-d-1} H(n-k-t) - \sum_{i \in I - \{d\}} h(n-2k+i) \\ &+ \sum_{i \in I} \sum_{t=1}^{s} b_t H(n-2k+i+t) \\ &\leq (q-1) \sum_{t=1}^{k-d} h(n-k-t) - \sum_{i \in I - \{d\}} h(n-2k+i). \end{split}$$

It is easy to see that

$$\begin{split} H'(n) &\geq h'(n-k) - \sum_{i \in I'} h'(n-2k+i) \\ &= (q-1) \sum_{t=1}^{k-d'} h'(n-k-t) - \sum_{i \in I' - \{d'\}} h'(n-2k+i) - \sum_{t=0}^{k-d'-1} H'(n-k-t). \end{split}$$

It follows that

$$H(n) - H'(n) \le (q-1) \sum_{t=1}^{k-d} h(n-k-t) - \sum_{i \in I - \{d\}} h(n-2k+i) - (q-1) \sum_{t=1}^{k-d'} h'(n-k-t) + \sum_{i \in I' - \{d'\}} h'(n-2k+i) + \sum_{t=0}^{k-d'-1} H'(n-k-t).$$
(2.24)

Suppose  $d' \leq d$ . One has

$$H(n) - H'(n) \le -h'(n - 2k + r) + \sum_{i=d+1}^{r-1} h(n - 2k + i) + \sum_{t=0}^{k-d'-1} H'(n - k - t)$$
  
$$\le -h'(n - 2k + r) + \sum_{i=d+1}^{r-1} h'(n - 2k + i) + \sum_{t=0}^{k-d'-1} H'(n - k - t)$$
  
$$\le -h'(n - 2k + d) + \sum_{t=0}^{k-d'-1} H'(n - k - t) \le 0,$$

using Corollary 2.4.6 and the fact that  $h'(n-2k+r) - (q-1) \sum_{t=1}^{r-d-1} h'(n-2k+r-t) \ge (q-1)h'(n-2k+d)$  since r-d-1 < k-s.

Suppose d' > d. If r = d then  $I = I' \cup \{d\}$ . Inequality (2.24) becomes

$$H(n) - H'(n) \le (q-1) \sum_{t=k-d'+1}^{k-d} h(n-k-t) - h'(n-2k+d') + \sum_{t=0}^{k-d'} H'(n-k-t) \le -h'(n-2k+d-1) + \sum_{t=0}^{k-d} H'(n-k-t) \le 0.$$

where we have used Corollary 2.4.6.

Assuming now that r > d' we add and subtract h'(n - 2k + d') to inequality (2.24) and use corollary 2.4.6 to obtain

$$H(n) - H'(n) \le (q-1) \sum_{t=k-r}^{k-d} h(n-k-t) - h(n-2k+r) - h(n-$$

$$(q-1)\sum_{t=k-r}^{k-d'} h'(n-k-t) + \sum_{t=r-1}^{d'} h'(n-2k+i) - h'(n-2k+d') + \sum_{t=0}^{k-d'-1} H'(n-k-t) \le \sum_{t=k-d'+1}^{k-d} h(n-k-t) - h'(n-2k+r) + \sum_{t=k-r+1}^{k-d'} h(n-k-t) \le 0.$$

Finally, if d' > r > d then  $I' \subset I \cap \{k - 1, \dots, r + 1\}$  and we have

$$H(n) - H'(n) \le (q-1) \sum_{t=k-d'+1}^{k-d} h(n-k-t) - h'(n-2k+d')$$
$$-h(n-2k+d) + \sum_{t=0}^{k-d'-1} H'(n-k-t) \le 0.$$

By combining statements prooved in this section one can deduce Theorems 1 and 2 for the k = k'. Indeed, let  $\Delta(n) = h(n) - h'(n)$ . Then  $\Delta(n) \leq 0$  for n < 4k, hence  $N \geq 4k$ . According to Lemma 2.4.3 one has  $\Delta(N+t) \geq q\Delta(N+t-1) \geq (q-1)\Delta(N+t-1)$  for  $0 \leq t \leq k-1$ , and by Corollary 2.4.3 this implies  $\Delta(N+k) \geq (q-1)\Delta(N+k-1)$ . By a simple inductive argument, Corollary 2.4.3 then implies that  $\Delta(n) \geq (q-1)\Delta(n-1)$  for any  $n \geq N$ . Theorem 2 follows from Theorem 1 by observing that  $P_w(n) = h(n+k)/q^{n+k}$ and likewise  $P_{w'}(n) = h'(n+k)/q^{n+k}$ . Finally Theorem 3 is an immediate consequence of Lemma 2.4.2.

# 2.5 A Proof of Theorems 1 and 2 when k is greater than k'

**Lemma 2.5.1.** Let k > k'. Then  $h(n) - q^{k-k'}h'(n-k+k') \le 0$  for  $n \le k+1$ .

 $\textit{Proof.} \ \ \text{Note that} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ k-k' < n < k \ \text{and} \ h(n) - q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n-k+k') = 0 \ \text{for} \ h(n) + q^{k-k'} h'(n) + q^{k-$ 

 $k + k') = 1 - q^{k-k'} < 0$  when n = k. When n = k + 1, for any  $0 \le m \le k - k'$  one has

$$\begin{split} h(k+1) - q^m h'(k'+1) &\leq q - q^{m+1} + q^m H'(k'+1) \\ &\leq -q^{m+1} + 2q^m \leq 0. \end{split}$$

Lemma 2.5.2. Let k > k' and N > k + 1. If  $h(n) - q^{k-k'}h'(n-k+k') \le 0$  for n < N, then  $H(n) - q^{k-k'}H'(n-k+k') \le 0$  for  $N \le n \le N+k$ .

*Proof.* For  $0 \le m \le k - k'$  one has

$$H(n) - q^{m}H'(n-m) \le h(n-k) - q^{m}(q-1)h'(n-k'-1-m)$$
$$\le h(n-k) - q^{m}h'(n-k-m),$$

and the result follows.

Note that in Lemma 2.5.2 the inequality  $H(n) - q^{k-k'}H'(n-k+k') \le 0$  is equivalent to  $q(h(n-1) - q^{k-k'}h'(n-k+k'-1)) \le h(n) - q^{n-k+k'}h'(n-k+k')$ .

Lemma 2.5.3. Let k > k' and  $n \ge 2k$ . If  $h(n-t) - q^{k-k'}h'(n-k+k'-t) \ge (q-1)(h(n-t-1) - q^{k-k'}h'(n-k+k'-t-1))$  for  $1 \le t \le k-1$  then  $h(n) - q^{k-k'}h'(n-k+k'-t) \ge (q-1)(h(n-1) - q^{k-k'}h'(n-k+k'))$ .

*Proof.* For any  $0 \le m \le k - k'$  have

$$\begin{split} h(n) - q^m h'(n-m) =& qh(n-1) - H(n) - q^{m+1}h'(n-m-1) + q^m H'(n-m) \\ =& q\left(h(n-1) - q^m h'(n-m-1)\right) + q^m H'(n-m) - H(n) \\ \geq& q\left(h(n-1) - q^m h'(n-m-1)\right) \\ & + q^m (q-1)h'(n-k'-m-1) - H(n) \\ \geq& q\left(h(n-1) - q^m h'(n-m-1)\right) \end{split}$$

$$+ q^{m}h'(n - k' - m - 1) - h(n - k)$$
  

$$\geq q (h(n - 1) - q^{m}h'(n - m - 1)) + q^{m}h'(n - k - m) - h(n - k)$$

Denote K = k - k'. With m = K we apply the inductive assumption to obtain

$$\begin{split} h(n) &- q^{m} h'(n-m) \\ \geq q \left( h(n-1) - q^{K} h'(n-K-1) \right) + q^{K} h'(n-k-K) - h(n-k) \\ \geq q \left( h(n-1) - q^{K} h'(n-K-1) \right) + q^{K} h'(n-1-K) - h(n-1) \\ = & (q-1) \left( h(n-1) - q^{K} h'(n-K-1) \right). \end{split}$$

The lemmas of this section combine to prove the main theorems when k > k' in the following way. Let  $\Delta(n) = h(n) - q^{k-k'}h'(n-k+k')$ . Then according to Lemma 2.5.3 one has  $\Delta(n) \le 0$  for  $n \le k + 1$  hence N > k + 1, which is the statement of Theorem 3. According to Lemma 2.5.2 one has  $\Delta(N + t) \ge q\Delta(N + t - 1) \ge (q - 1)\Delta(N + t - 1)$  for  $0 \le t \le k - 1$ , and by Lemma 2.5.3 this implies  $\Delta(N + k) \ge (q - 1)\Delta(N + k - 1)$ . By a simple inductive argument, Lemma 2.5.3 then implies that  $\Delta(n) \ge (q - 1)\Delta(n - 1)$  for any  $n \ge N$ . Dividing  $\Delta(n)$  by  $q^{n-k}$  then yields Theorem 2.

Observe that Lemmas 2.5.1, 2.5.2, and 2.5.3 hold if everywhere in their statements we replace k - k' with any m satisfying  $0 \le m \le k - k'$ . Theorem 1 is a consequence of setting m = 0.

# 2.6 An Upper Bound for Delta when s equals s'

We will provide an upper bound for  $\Delta(n)$  when  $2k < n \le 4k$ . Viewing  $\Delta(n)$  as a function of the values  $b_i$  and  $b'_i$  for i < r, we will show that if  $b_i = 0$  then  $\Delta(b_i+1, n) - \Delta(b_i, n) \le 0$ . One can also show that if  $b'_i = 1$  then  $\Delta(b'_i - 1, n) - \Delta(b'_i, n) \le 0$ . Because of the almost complete redundancy in these calculations, we will only display the former case.

Let

$$\tilde{b}_t = \begin{cases} 1 & b_t = 1 \text{ and } t \in I \\ 0 & \text{otherwise} \end{cases}$$

and

$$\delta(n) = \sum_{t=1}^{3k-n-1} b_t \tilde{b}_{3k-n-t} - b'_t \tilde{b}'_{3k-n-t}.$$

For  $2k \le n < 3k - s$  one has

$$H(n) - H'(n) = -\delta(n).$$

For  $2k + (k - s) \le n < \min\{2k + 2(k - s), 3k - r\}$  one has

$$H(n) - H'(n) = -\delta(n) + \delta(n - k + s).$$

For  $2k \le n < 3k - r - 1$  we thus assume that

$$H(n) - H'(n) = -\delta(n) + \delta(n - k + s)$$

with the convention that  $\delta(n) = 0$  when n < 2k.

Let n < 3k - r. If t > r and  $t \notin S$ , one has n - k + t < 2k - r + t < 3k - s - r, hence H(n - k + t) - H'(n - k + t) = 0. Let  $p = \lfloor \frac{n-2k}{k-s} \rfloor$ . One then has

$$H(n) - H'(n) = -\delta(n) - \sum_{t=3k-n}^{s} b_i (H(n-k+t) - H'(n-k+t))$$
$$= -\delta(n) - \sum_{t=1}^{p} \left( H(n-t(k-s)) - H'(n-t(k-s)) \right)$$

$$-\sum_{t \in (I-\{s\}) \cap \{r+1,\dots,m\}} (H(n-k+t) - H'(n-k+t))$$
  
=  $-\delta(n) - \sum_{l=1}^{p} \left( -\delta(n-l(k-s)) + \delta(n-(l+1)(k-s)) \right)$   
=  $-\delta(n) + \delta(n-k+s),$ 

where we observe that  $n - (p+1)(k-s) \le 2k$ . It follows that for n < 3k - r one has

$$H(n) - H'(n) = -\delta(n) + \delta(n - k + s).$$
(2.25)

For 2k < n < 3k - r by using (2.25) one thus has

$$\Delta(n) = -q^{n-2k} \sum_{t=1}^{r} q^t (\tilde{b}_t - \tilde{b}'_t) + \sum_{t=2k}^{n} q^{n-t} \delta(t) - \sum_{t=3k-s}^{n} q^{n-t} \delta(t-k+s), \qquad (2.26)$$

where we have used the fact that

$$\Delta(2k) = -\sum_{t=1}^{r} q^t (\tilde{b}_t - \tilde{b}'_t)$$

when s = s'.

For  $n \ge k$  let us denote by  $h^*(n)$  the solution to the recurrence relation  $h^*(n) = \sum_{t=1}^k b_t^*(qh^*(n+t-1)-h^*(n+t))$  where

$$b_t^* = \begin{cases} b_t & t \neq i \\ 1 & t = i \end{cases}$$

subject to the initial conditions  $h^*(n) = 0$  for n < k and  $h^*(k) = 1$ . Let  $H^*(n) = qh^*(n-1) - h^*(n)$ .

Denote

$$\delta^{*}(t) = \tilde{b}_{3k-t-i}^{*} + b_{3k-t-i}^{*}$$

and observe that  $\delta^*(t) = h^*(t) - h(t)$ . We will also denote

$$\Delta^*(n) = h^*(n) - h(n).$$

It is easy to see that

$$\delta^{*}(t) \begin{cases} = 0, \quad t < 3k - i - s \\ = 2, \quad t = 3k - i - s \\ = 0, \quad t = 3k - i - s + 1, \end{cases}$$

$$0 \le \delta^{*}(t) \le 2 \text{ for } 3k - i - s + 1 < t \le 3k - 1.$$

$$(2.27)$$

For n < 3k - s equality (2.26) becomes

$$\Delta^*(n) = -q^{n-2k+i} + \sum_{t=2k}^n q^{n-t} \left( \tilde{b}^*_{3k-t-i} + b^*_{3k-t-i} \right)$$
$$= -q^{n-2k+i} + \sum_{t=3k-s-i}^n q^{n-t} \left( \tilde{b}^*_{3k-t-i} + b^*_{3k-t-i} \right) < 0,$$

where we have used the fact that  $i \le k - s - 2$ . If  $3k - s \le n < 3k - i$  then

$$\Delta^{*}(n) = -q^{n-2k+i} + \sum_{t=2k}^{n} q^{n-t} \left( \tilde{b}_{3k-t-i}^{*} + b_{3k-t-i}^{*} \right) - \sum_{t=3k-s}^{n} q^{n-t} \left( \tilde{b}_{3k-t-i+k-s}^{*} + b_{3k-t-i+k-s}^{*} \right) < 0.$$
(2.28)

Let  $3k - i \le n \le 3k$ . One has

$$\Delta^{*}(n) \leq -q^{n-2k+i} + \sum_{t=2k}^{3k-i-1} q^{n-t} \left( \tilde{b}_{3k-t-i}^{*} + b_{3k-t-i}^{*} \right) - \sum_{t=3k-i}^{n} q^{n-t} \left( H^{*}(t) - H(t) \right) = -q^{n-2k+i} + \sum_{t=2k}^{3k-i-1} q^{n-t} \left( \tilde{b}_{3k-t-i}^{*} + b_{3k-t-i}^{*} \right) - \sum_{t=3k-i}^{n} q^{n-t} \Delta^{*}(t-k) + \sum_{t=3k-i}^{n} q^{n-t} H^{*}(t-k+i) + \sum_{t=3k-i}^{n} q^{n-t} \sum_{j=1}^{s} b_{j} \left( H^{*}(t-k+j) - H(t-k+j) \right).$$
(2.29)

Note that  $t - k + j \le 2k + s < 3k - i$  hence  $H^*(t - k + j) - H(t - k + j) = -\delta^*(t - k + j) + \delta^*(t - 2k + j + s)$  when  $t - k + j \ge 2k$ .

One has

$$\sum_{t=3k-j}^{n} q^{n-t} b^*_{4k-t-j-i} - \sum_{t=3k-j+(k-s)}^{n} q^{n-t} b^*_{4k-t-j-i+(k-s)}$$
$$= \sum_{t=3k-j}^{n} q^{n-t} b^*_{4k-t-j-i} - \sum_{t=3k-j}^{n-k+s} q^{n-t-k+s} b^*_{4k-t-j-i} \ge 0$$

and similarly

$$\sum_{t=3k-j}^{n} q^{n-t} \tilde{b}_{4k-t-j-i}^* - \sum_{t=3k-j+(k-s)}^{n} q^{n-t} \tilde{b}_{4k-t-j-i+(k-s)}^* \ge 0.$$

It follows that

$$\sum_{t=3k-j}^{n} q^{n-t} (H^*(t-k+j) - H(t-k+j))$$

$$= \sum_{t=3k-j}^{n} q^{n-t} \delta^*(t-k+j) - \sum_{t=3k-j+(k-s)}^{n} q^{n-t} \delta^*(t-k+j-(k-s)) \ge 0.$$
(2.30)

Applying (2.30) one has

$$\sum_{t=3k-i}^{n} q^{n-t} \sum_{j=1}^{s} b_j \left( H^*(t-k+j) - H(t-k+j) \right)$$

$$= \sum_{j=1}^{i-1} b_j \sum_{t=3k-i}^{3k-j-1} q^{n-t} \left( \tilde{b}_{3k-t-j}^* - \tilde{b}_{3k-t-j} \right) - \sum_{j=1}^{s} \sum_{t=3k-j}^{n} q^{n-t} (H^*(t-k+j) - H(t-k+j))$$

$$\leq \sum_{j=1}^{i-1} b_j \sum_{t=3k-i}^{3k-j-1} q^{n-t} \left( \tilde{b}_{3k-t-j}^* - \tilde{b}_{3k-t-j} \right)$$
(2.31)

for  $n \leq 3k$ .

For  $3k - i \le t < 3k$  note that

$$\Delta^*(t-k) = -\sum_{l=3k-t}^{i} q^{t-3k+l} \left(b_l^* - b_l\right)$$
(2.32)

and recall

$$\Delta^*(2k) = -\sum_{l=1}^{i} q^l (b_l^* - b_l),$$

whence  $\Delta^*(t-k) = -q^{t-3k+i}$  for  $3k-i \le t \le 3k$ . Using  $H^*(t-k+i) \le q^{t-3k+i}$  for  $t-k+i \ge 2k$  and (2.31), equality (2.29) becomes

$$\Delta^{*}(n) \leq -q^{n-2k+i} + \sum_{t=2k}^{3k-i-1} q^{n-t} \left( \tilde{b}_{3k-t-i}^{*} + b_{3k-t-i}^{*} \right)$$

$$+ \sum_{t=3k-i}^{n} q^{n-3k+i} + \sum_{t=3k-i}^{n} q^{n-3k+i} + \sum_{j=1}^{i-1} b_{j} \sum_{t=3k-i}^{3k-j-1} q^{n-t} \left( \tilde{b}_{3k-t-j}^{*} - \tilde{b}_{3k-t-j} \right)$$

$$\leq -q^{n-2k+i} + 2 \sum_{t=3k-s-i}^{3k-i-1} q^{n-t} + 2(i+1)q^{n-3k+i} + q^{n-3k+2i}$$

$$\leq -q^{n-2k+i} + q^{n-3k+s+i+2} + q^{n-3k+2i+1} + q^{n-3k+2i} \leq 0$$

$$(2.33)$$

where we observe that  $\tilde{b}_{3k-t-j}^* - \tilde{b}_{3k-t-j} = 1$  if and only if t = 3k - i - j and where we

have used the facts  $i < r \le k - s - 2$  and  $2(i + 1) \le q^{i+1}$ .

Let 3k < n < 4k. Using (2.17) one has

$$-\sum_{t=3k+1}^{n} q^{n-t} \left( H^*(t) - H(t) \right) = -\sum_{t=3k+1}^{n} q^{n-t} \Delta^*(t-k) + \sum_{t=3k+1}^{n} \sum_{j \in I} \Delta^*(t-2k+j)$$
  
$$-\sum_{t=3k+1}^{n} q^{n-t} \sum_{j \in I} \sum_{l=1}^{k-j} b_l \left( H^*(t-2k+j+l) - H(t-2k+j+l) \right)$$
  
$$+\sum_{t=3k+1}^{n} q^{n-t} H^*(t-k+i) - \sum_{t=3k+1}^{n} \sum_{j \in I} q^{n-t} H^*(t-2k+j+i).$$
  
(2.34)

For fixed j and  $u \leq 4k-j-l-1$  one has

$$-\sum_{l=1}^{k-j} b_l \sum_{t=3k+1}^{u} q^{n-t} \left( H^*(t-2k+j+l) - H(t-2k+j+l) \right)$$

$$= -\sum_{l=1}^{k-j} b_l \sum_{t=3k+1}^{u} q^{n-t} \left( \tilde{b}^*_{4k-t-j-l} - \tilde{b}_{4k-t-j-l} \right) \le 0,$$
(2.35)

observing that  $\tilde{b}_{\iota}^* \geq \tilde{b}_{\iota}$ . For  $4k - j - l - 1 \leq u \leq 5k - j - l - i - 1$  one also has

$$-\sum_{l=1}^{k-j}\sum_{t=4k-j-l-1}^{u}q^{n-t}\left(H^{*}(t-2k+j+l)-H(t-2k+j+l)\right)$$

$$=\sum_{l=1}^{k-j}\sum_{t=4k-j-l-1}^{u}q^{n-t}\left(\delta^{*}(t-2k+j+l)-\delta^{*}(t-2k+j+l-k+s)\right) \qquad (2.36)$$

$$\leq\sum_{l=1}^{k-j}\sum_{t=5k-j-l-s-i}^{u}q^{n-t}\delta^{*}(t-2k+j+l)\leq 2q^{n-4k+i+s+2}.$$

For  $3k - i \le n \le 3k$  one has

$$H^*(n) - H(n) = \Delta^*(n-k) - \sum_{t=1}^s b_t \left( H^*(n-k+t) - H(n-k+t) \right) - H^*(n-k+i)$$

$$\geq \Delta^*(n-k) - \sum_{t=1}^s \delta^*(n-2k+t+s) - H^*(n-k+i)$$
  
$$\geq -q^{n-3k+i} - 2s - H^*(n-k+i).$$

For  $n \geq 4k-i$  one thus has

$$-\sum_{l=1}^{k-j}\sum_{t=5k-j-l-i}^{n}q^{n-t}\left(H^{*}(t-2k+j+l)-H(t-2k+j+l)\right)$$

$$\leq -\sum_{l=1}^{k-j}\sum_{t=5k-j-l-i}^{n}q^{n-t}\left(-q^{t-5k+j+l+i}-2s-H^{*}(t-3k+j+l+i)\right)$$

$$\leq q^{n-4k+2i}+q^{n-4k+s+i+2}+\sum_{l=1}^{k-j}\left(\sum_{t=5k-j-l-i}^{5k-j-l-i-1}q^{n-t}+\sum_{t=5k-j-l-i}^{n}q^{n-5k+j+l+i}\right)$$

$$\leq q^{n-4k+2i}+q^{n-4k+s+i+2}+q^{n-4k+i+2}+q^{n-4k+2i}$$

$$\leq 2q^{n-3k-4}+q^{n-3k-1}+q^{n-3k-3}\leq q^{n-3k-1}+q^{n-3k-2}+q^{n-3k-3},$$

$$(2.37)$$

where we have applied (2.32) and used the inequalities

$$i \le q^{i-1}, \quad i < r, \quad r \le k - s - 2, \quad r \le \frac{k}{2} - 1, \quad s \le k - 3.$$
 (2.38)

For n < 4k - i

$$-\sum_{l=1}^{k-j}\sum_{t=5k-j-l-i}^{n}q^{n-t}\left(H^*(t-2k+j+l)-H(t-2k+j+l)\right) = 0$$
(2.39)

since the former sum is empty. Using (2.35), (2.36), and (2.39), for 3k < n < 4k - i one has

$$-\sum_{t=3k+1}^{n} q^{n-t} \sum_{j\in I} \sum_{l=1}^{k-j} b_l \left( H^*(t-2k+j+l) - H(t-2k+j+l) \right) \le \sum_{j\in I} 2q^{n-4k+s+i+2}.$$
(2.40)

For any 3k < n < 4k note that

$$\sum_{j \in I} \sum_{t=3k+1}^{n} q^{n-t} H^*(t-2k+j+i)$$

$$= \sum_{j \in I} \left( \sum_{t=4k-j-i-s}^{4k-j-i-1} q^{n-t} \tilde{b}^*_{4k-t-j-i} + \sum_{t=4k-j-i}^{n} q^{n-t} H^*(t-2k+j+i) \right)$$
(2.41)
$$\leq \sum_{j \in I} \left( q^{n-4k+j+i+s+1} + (n-3k)q^{n-4k+j+i} \right) \leq q^{n-3k+s-2} + (n-3k)q^{n-3k-2}.$$

For 3k < n < 4k - i one has  $\Delta^*(t - k) \ge -q^{t-3k+i}$ . Applying inequalities (2.40) and (2.41) to (2.34) we have

$$\begin{split} &-\sum_{t=3k+1}^n q^{n-t} \left( H^*(t) - H(t) \right) \leq -\sum_{t=3k+1}^n q^{n-t} \Delta^*(t-k) + (k-s) 2q^{n-4k+s+i+2k+1} \\ &+ (n-3k)q^{n-3k+i} + (n-3k)q^{n-3k-2} + q^{n-3k+s-2k+1} \\ &\leq (n-3k-1)q^{n-3k+i} + (k-s)q^{n-4k+s+i+3} + (n-3k)q^{n-3k+i} \\ &+ (n-3k)q^{n-3k-2} + q^{n-3k+s-2k+1} \\ &\leq q^{n-3k+i+k/2} + q^{n-3k+i+2k+1} + q^{n-3k+i+k/2k+1} + q^{n-3k+k/2k+1} + q^{n-3k+k/2k+1} \\ &\leq 4q^{n-2k-3k+1} + q^{n-2k-2k+1}, \end{split}$$

where we have used the inequality  $n - 3k \le k - 1 \le q^{k/2}$ , inequalities (2.38), and the fact that  $k \ge 5$  when s = s'.

Similar to (2.33) one has

$$q^{n-2k}\Delta^*(2k) - \sum_{t=2k}^{3k-1} q^{n-t}(H^*(t) - H(t))$$
  
$$\leq -q^{n-2k+i} + q^{n-3k+s+i+2} + q^{n-3k+2i+1} + q^{n-3k+2i}.$$

It follows that for 3k < n < 4k - i we have

$$\Delta^*(n) \le q^{n-2k} \left( -q^i + q^{-1} + q^{-5} + q^{-6} + 4q^{-3} + q^{-5} \right) \le 0,$$

where we have again used the inequalities (2.38).

For  $3k - i \le n \le 3k$  it is easy to see that

$$\begin{split} \Delta^*(n) &\geq -q^{n-2k+i} - \sum_{t=3k-i}^n q^{n-t} (H^*(t) - H(t)) \\ &\geq -q^{n-2k+i} - (n-3k+i)q^{n-2k} \\ &\geq -q^{n-2k+i} - q^{n-2k+i}. \end{split}$$

For  $4k - i \le n < 4k$  one thus has

$$-\sum_{t=3k+1}^{n} q^{n-t} \left( H^*(t) - H(t) \right) \le 4q^{n-2k-3} + q^{n-2k-5} + \sum_{t=4k-i}^{n} q^{n-3k+i} + q^{n-3k-1} + q^{n-3k-2} + q^{n-3k-3} \le 4q^{n-2k-3} + q^{n-2k-5} + q^{n-3k+2i-1} + q^{n-3k} \le 4q^{n-2k-3} + 3q^{n-2k-5}$$

where we have used (2.37).

For  $4k - i \le n < 4k$  one thus has

$$\Delta^*(n) \le q^{n-2k} \left( -q^i + q^{-1} + q^{-5} + q^{-6} + 4q^{-3} + 3q^{-5} \right) \le 0.$$

Given w and  $\iota \in I - \{s\}$ , let  $h_{\iota}(n)$  be the solution to the recurrence relation defined by

$$h_{\iota}(n) = \sum_{t=1}^{k} c_{t}(qh_{\iota}(n-t-1) - h_{\iota}(n-t)), \quad c_{t} = \begin{cases} b_{t} & t > \iota \\ 0 & t = \iota \\ 1 & t < \iota \end{cases}$$

and  $h^{\iota}(n)$  the solution to

$$h^{\iota}(n) = \sum_{t=1}^{k} c_t (qh^{\iota}(n-t-1) - h^{\iota}(n-t)), \quad c_t = \begin{cases} b_t & t > \iota \\ 1 & t = \iota \\ 0 & t < \iota \end{cases}$$

We have shown that  $\Delta(b_i + 1, n) \leq \Delta(b_i, n)$  for  $2k \leq n < 4k$ . As we remarked, with minimal alterations to the calculations of this section one can show the inequality  $\Delta(b'_i - 1, n) \leq \Delta(b'_i, n)$ . Thus  $\Delta(n) \leq \Delta_r(n)$  for  $2k \leq n < 4k$  where  $\Delta_r(n) = h^r(n) - h_r(n)$ .

## 2.7 The Upper Bound is Negative

We will show that  $\tilde{\Delta}(n) \leq 0$  for  $2k \leq n < 4k$ . Throughout this section we will let  $h(n) = h^r(n)$  and  $h'(n) = h_r(n)$  to avoid burdening the notation.

For t < 3k - r one has

$$\begin{split} \delta(t) &= \tilde{b}_{3k-t-r} - \sum_{l=1}^{r-1} \tilde{b}'_{3k-t-l} + \sum_{l=r+1}^{3k-t-1} b_l \left( \tilde{b}_{3k-t-l} - \tilde{b}'_{3k-t-l} \right) \\ &= \tilde{b}_{3k-t-r} - \sum_{l=1}^{r-1} \tilde{b}'_{3k-t-l} + \sum_{l=r+1}^{3k-t-r-1} b_l \left( \tilde{b}_{3k-t-l} - \tilde{b}'_{3k-t-l} \right) + b_{3k-t-r} - \sum_{l=3k-t-r+1}^{3k-t-1} b_l \\ &= \tilde{b}_{3k-t-r} - \sum_{l=1}^{r-1} \tilde{b}'_{3k-t-l} + b_{3k-t-r} - \sum_{l=3k-t-r+1}^{3k-t-1} b_l \\ &= \tilde{b}_{3k-t-r} - \sum_{l=1}^{r-1} \tilde{b}'_{3k-t-l} + b_{3k-t-r} - \sum_{l=1}^{r-1} b_{3k-t-l} . \end{split}$$

It is thus easy to see that

$$\delta(t) \begin{cases} = 0, \quad t < 3k - s - r \\ = 2, \quad t = 3k - s - r \\ = -2, \quad t = 3k - s - r + 1 \end{cases} \begin{cases} \le 2, \quad t < 3k - r \\ \ge -2, \quad t < 2k + s - r \\ \ge -2(r - 1), \quad 2k + s - r \le t < 3k - r \end{cases}$$

$$(2.42)$$

Using (2.42), for n < 3k - r one thus has

$$-\sum_{t=3k-s}^{n} q^{n-t}\delta(t-k+s) \le 0$$

and

$$\sum_{t=2k}^{n} q^{n-t} \delta(t) \le 2q^{n-3k+s+r}.$$

Using (2.26) and the equality  $\Delta(2k) = -2$ , for  $2k \le n < 3k - r$  one thus has

$$\Delta(n) \le -q^{n-2k} \Delta(2k) + 2q^{n-3k+s+r} \le -2\left(q^{n-2k} - q^{n-3k+s+r}\right) < 0.$$

Let  $3k - r \le n \le 3k$ . One has

$$\Delta(n) = q^{n-3k+r+1}\Delta(3k-r-1) - \sum_{t=3k-r}^{n} q^{n-t}(H(t) - H'(t))$$
  
=  $q^{n-3k+r+1}\Delta(3k-r-1) - \sum_{t=3k-r}^{n} q^{n-t}\Delta(t-k)$  (2.43)  
+  $\sum_{t=3k-r}^{n} q^{n-t}\sum_{j=1}^{s} \left( b_j H(t-k+j) - b'_j H'(t-k+j) \right).$ 

Note that

$$\sum_{t=3k-r}^{n} q^{n-t} \sum_{j=1}^{s} \left( b_{j}H(t-k+j) - b_{j}'H'(t-k+j) \right)$$

$$= \sum_{t=3k-r}^{n} \left( q^{n-t}H(t-k+r) - \sum_{j=1}^{r-1} q^{n-t}H'(t-k+j) \right)$$

$$+ \sum_{j=r+1}^{s} b_{j} \sum_{t=3k-r}^{n} q^{n-t} \left( H(t-k+j) - H'(t-k+j) \right)$$

$$\leq \sum_{t=3k-r}^{n} q^{n-t}H(t-k+r) + \sum_{j=r+1}^{s} b_{j} \sum_{t=3k-r}^{n} q^{n-t} \left( H(t-k+j) - H'(t-k+j) \right).$$

For  $r < j \le s$  and  $3k - r \le t \le n$  one has 2k < t - k + j < 3k - r, and again using (2.42) we have

$$\begin{split} &\sum_{j=r+1}^{s} b_j \sum_{t=3k-r}^{n} q^{n-t} \left( H(t-k+j) - H'(t-k+j) \right) \\ &= -\sum_{j=r+1}^{s} b_j \sum_{t=3k-r}^{n} q^{n-t} \left( \delta(t-k+j) - \delta(t-2k+j+s) \right) \\ &\leq 2(r-1) \sum_{j=r+1}^{s} b_j q^{n-3k+r+1} + 2 \sum_{j=r+1}^{s} b_j q^{n-5k+2s+r+j} \\ &\leq 2(r-1) q^{n-3k+s} + q^{n-5k+3s+r+2} \leq q^{n-3k+s+r-1} + q^{n-4k+2s} \\ &\leq q^{n-3k+s+r-1} + q^{n-3k+s-3}, \end{split}$$

where we have applied the inequalities  $r + s \le k - 2$  and  $s \le k - 3$ . Inequality (2.43) thus

becomes

$$\begin{aligned} \Delta(n) &= q^{n-3k+r+1} \Delta(3k-r-1) - \sum_{t=3k-r}^{n} q^{n-t} (H(t) - H'(t)) \\ &\leq q^{n-3k+r+1} \Delta(3k-r-1) - \sum_{t=3k-r}^{n} q^{n-t} \Delta(t-k) + q^{n-3k} ((r+1)q^r + q^{s+r-1} + q^{s-3}) \\ &\leq -2q^{n-2k} + 2q^{n-3k+r+s} + \sum_{t=3k-r}^{n} q^{n-t} + q^{n-3k} (q^{2r} + q^{s+r-1} + q^{s-3}) \\ &\leq -2q^{n-2k} + q^{n-3k} (q^{s+r+1} + q^{r+1} + q^{2r} + q^{s+r-1} + q^{s-3}) \\ &\leq -q^{n-2k}, \end{aligned}$$

$$(2.44)$$

where we have used the inequality  $\Delta(3k - r - 1) \leq -2(q^{k-r-1} - q^{s-1})$  and the fact that  $\Delta(n) = -1$  for  $2k - r \leq n \leq 2k$ .

Let 3k < n < 4k. Denote  $I_t = I \cap \{t, \dots, s\}$ . One has

$$-\sum_{t=3k+1}^{n} q^{n-t} (H(t) - H'(t)) = -\sum_{t=3k+1}^{n} q^{n-t} \Delta(t-k) + \sum_{t=3k+1}^{n} q^{n-t} \sum_{j \in I_{r+1}} \Delta(t-2k+j)$$
$$-\sum_{t=3k+1}^{n} q^{n-t} \sum_{j \in I_{r+1}} \sum_{l=1}^{k-j} (b_l H(t-2k+j+l) - b'_l H'(t-2k+j+l))$$
$$+\sum_{t=3k+1}^{n} q^{n-t} H(t-k+r) - \sum_{j=1}^{r-1} \sum_{t=3k+1}^{n} q^{n-t} H'(t-k+j),$$

hence

$$-\sum_{t=3k+1}^{n} q^{n-t} (H(t) - H'(t)) \leq -\sum_{t=3k+1}^{n} q^{n-t} \Delta(t-k) + \sum_{t=3k+1}^{n} q^{n-t} H(t-k+r) -\sum_{t=3k+1}^{n} q^{n-t} \sum_{j\in I_{r+1}} \sum_{l=1}^{k-j} \left( b_l H(t-2k+j+l) - b'_l H'(t-2k+j+l) \right).$$
(2.45)

Let n < 4k - r. Note that t - 2k + j + l < 3k - r. For fixed j, if  $r < l \le k - j$  one has

$$\begin{split} &-\sum_{t=3k+1}^{n}q^{n-t}\left(b_{l}H(t-2k+j+l)-b_{l}'H'(t-2k+j+l)\right)\\ &=-b_{l}\sum_{t=3k+1}^{n}q^{n-t}\left(H(t-2k+j+l)-H'(t-2k+j+l)\right)\\ &\leq -b_{l}\sum_{t=3k+1}^{4k-j-l-1}q^{n-t}\left(\tilde{b}_{4k-t-j-l}-\tilde{b}_{4k-t-j-l}'\right)+b_{l}\sum_{t=4k-j-l}^{n}q^{n-t}\delta(t-2k+j+l)\\ &-b_{l}\sum_{t=4k-j-l}^{n}q^{n-t}\delta(t-3k+j+l+s). \end{split}$$

For any  $u \leq 4k - j - l - 1$  observe that

$$-\sum_{j\in I_{r+1}}\sum_{l=r+1}^{k-j}b_l\sum_{t=3k+1}^{u}q^{n-t}\left(\tilde{b}_{4k-t-j-l}-\tilde{b}'_{4k-t-j-l}\right)$$
$$=-\sum_{j\in I_{r+1}}\sum_{l=r+1}^{k-j}b_l\sum_{t=4k-j-l-r}^{u}q^{n-t}\left(\tilde{b}_{4k-t-j-l}-\tilde{b}'_{4k-t-j-l}\right)$$
$$=-\sum_{j\in I_{r+1}}\sum_{l=r+1}^{k-j}b_l\sum_{t=4k-j-l-u}^{r}q^{n-4k+j+l+t}\left(\tilde{b}_t-\tilde{b}'_t\right) \le 0.$$

Similarly, for any  $u \leq 5k - j - l - r - 1$  one has

$$-\sum_{j\in I_{r+1}}\sum_{l=1}^{k-j}b_l\sum_{t=4k-j-l}^{u}q^{n-t}\delta(t-3k+j+l+s)\leq 0.$$

It follows that

$$-\sum_{t=3k+1}^{n} q^{n-t} \sum_{j\in I_{r+1}} \sum_{l=r+1}^{k-j} (b_l H(t-2k+j+l) - b'_l H'(t-2k+j+l))$$

$$\leq \sum_{j\in I_{r+1}} \sum_{l=r+1}^{k-j} b_l \sum_{t=4k-j-l}^{n} q^{n-t} \delta(t-2k+j+l).$$
(2.46)

Noting that  $r < k - s \le k - j$  for any  $j \in I$ , one has

$$\begin{split} &-\sum_{t=3k+1}^{n} q^{n-t} \sum_{j \in I_{r+1}} \sum_{l=1}^{r} \left( b_l H(t-2k+j+l) - b_l' H'(t-2k+j+l) \right) \\ &= -\sum_{j \in I_{r+1}} \left( \sum_{t=3k+1}^{4k-j-r-1} q^{n-t} \tilde{b}_{4k-t-j-r} - \sum_{l=1}^{r-1} \sum_{t=3k+1}^{4k-j-l-1} q^{n-t} \tilde{b}_{4k-t-j-l}' \right) \\ &- \sum_{j \in I_{r+1}} \left( \sum_{t=4k-j-r}^{n} q^{n-t} H(t-2k+j+r) - \sum_{l=1}^{r-1} \sum_{t=4k-j-l}^{n} q^{n-t} H'(t-2k+j+l) \right) \\ &\leq \sum_{j \in I_{r+1}} \sum_{l=1}^{r-1} \sum_{t=3k+1}^{4k-j-l-1} q^{n-t} \tilde{b}_{4k-t-j-l}' \\ &- \sum_{j \in I_{r+1}} \sum_{t=4k-j-r}^{n} q^{n-t} \left( H(t-2k+j+r) - H'(t-2k+j+r) \right). \end{split}$$

It is easy to see that

$$-\sum_{j\in I_{r+1}}\sum_{t=4k-j-r}^{n}q^{n-t}\left(H(t-2k+j+r)-H'(t-2k+j+r)\right)$$
$$\leq \sum_{j\in I_{r+1}}\sum_{t=4k-j-r}^{n}q^{n-t}\delta(t-2k+j+r).$$

We thus have

$$-\sum_{t=3k+1}^{n} q^{n-t} \sum_{j\in I_{r+1}} \sum_{l=1}^{r} \left( b_l H(t-2k+j+l) - b'_l H'(t-2k+j+l) \right)$$

$$\leq \sum_{j\in I_{r+1}} \sum_{l=1}^{r-1} \sum_{t=3k+1}^{4k-j-l-1} q^{n-t} \tilde{b}'_{4k-t-j-l} + \sum_{j\in I_{r+1}} \sum_{t=4k-j-r}^{n} q^{n-t} \delta(t-2k+j+r).$$
(2.47)

Using (2.46) and (2.47) we have

$$-\sum_{t=3k+1}^{n}\sum_{j\in I_{r+1}}\sum_{l=1}^{k-j}q^{n-t}\left(b_{l}H(t-2k+j+l)-b_{l}'H'(t-2k+j+l)\right)$$

$$\leq\sum_{j\in I_{r+1}}\sum_{l=r}^{k-j}b_{l}\sum_{t=5k-j-l-s-r}^{n}q^{n-t}\delta(t-2k+j+l)+\sum_{j}\sum_{l=1}^{r-1}\sum_{t=4k-j-l-s}^{4k-j-l-1}q^{n-t}\tilde{b}_{4k-t-j-l}'$$

$$\leq 2\sum_{j}\sum_{l=1}^{k-j}q^{n-5k+s+r+j+l}+\sum_{j}\sum_{l=1}^{r-1}q^{n-4k+s+j+l+1}$$

$$\leq 2\sum_{j}q^{n-4k+s+r+1}+\sum_{j}q^{n-4k+s+j+r+1}\leq q^{k-s-r-1}q^{n-4k+s+r+1}+q^{n-4k+2s+r+2}$$

$$\leq q^{n-3k}+q^{n-3k+s},$$
(2.48)

using the fact that  $2|I_{r+1}| \le 2(k - s - r - 1) \le q^{k - s - r - 1}$ .

For 2k < n < 3k - r, using equality (2.26) we easily obtain the lower bound

$$\begin{split} \Delta(n) &= -q^{n-2k} \Delta(2k) + \sum_{t=2k}^{n} q^{n-t} \delta(t) - \sum_{t=2k}^{n-k+s} q^{n-t-k+s} \delta(t) \\ &\geq -2q^{n-2k} + \sum_{t=n-k+s+1}^{n} q^{n-t} \delta(t). \end{split}$$

If 3k - s - r > n - k + s then  $\sum_{t=n-k+s+1}^{n} q^{n-t} \delta(t) \ge 0$ . If  $3k - s - r \le n - k + s$ then  $\sum_{t=2k}^{n} q^{n-t} \delta(t) \ge 0$  and  $-\sum_{t=2k}^{n-k+s} q^{n-t-k+s} \delta(t) \ge -2q^{n-4k+2s+r}$ . We thus obtain the lower bound

$$\Delta(n) \ge -2q^{n-2k} - 2q^{n-4k+2s+r}.$$
(2.49)

Applying (2.48) and (2.49) to (2.45) one has

$$-\sum_{t=3k+1}^{n} q^{n-t} (H(t) - H'(t)) \le -\sum_{t=3k+1}^{n} q^{n-t} \Delta(t-k) + \sum_{t=3k+1}^{n} q^{n-3k+r} + q^{n-3k} + q^{n-3k+s}$$

$$\leq 2 \sum_{t=3k+1}^{n} q^{n-3k} + 2 \sum_{t=3k+1}^{n} q^{n-5k+2s+r} + (k-r-1)q^{n-3k+r} + q^{n-3k} + q^{n-3k+s}$$

$$\leq 2(k-r-1)q^{n-3k} + 2(k-r-1)q^{n-5k+2s+r} + q^{n-2k-2} + q^{n-3k} + q^{n-3k+s}$$

$$\leq q^{n-2k-r-1} + q^{n-4k+2s-1} + q^{n-2k-2} + q^{n-3k} + q^{n-3k+s}$$

$$\leq 2q^{n-2k-2} + q^{n-2k-7} + q^{n-3k} + q^{n-2k-3}.$$

One thus has

$$\Delta(n) \le q^{n-2k}(-1+q^{-1}+q^{-7}+q^{-k}+q^{-3}) \le 0.$$

Let  $4k - r \le n < 4k$ . By calculations similar to those above, one has

$$-\sum_{j\in I_{r+1}}\sum_{l=1}^{k-j}\sum_{t=3k+1}^{n}q^{n-t}\left(b_{l}H(t-2k+j+l)-b_{l}'H'(t-2k+j+l)\right)$$

$$\leq \sum_{j\in I_{r+1}}\sum_{l=1}^{r-1}\sum_{t=3k+1}^{4k-j-l-1}q^{n-t}\tilde{b}_{4k-t-j-l}' + \sum_{j\in I_{r+1}}\sum_{l=r}^{k-j}b_{l}\sum_{t=4k-j-l}^{5k-r-j-l-1}q^{n-t}\delta(t-2k+j+l)$$

$$-\sum_{j\in I_{r+1}}\sum_{l=r}^{k-j}b_{l}\sum_{t=5k-r-j-l}^{n}q^{n-t}\left(H(t-2k+j+l)-H'(t-2k+j+l)\right).$$

For  $3k - r \le n < 3k$  observe that

$$H(n) - H'(n) \ge \Delta(n-k) - H(n-k+r) + \sum_{t=r+1}^{s} (\delta(n-k+t) - \delta(n-2k+t+s))$$
$$\ge -2 - q^{n-3k+r} + \sum_{t=r+1}^{s} (\delta(n-k+t) - \delta(n-2k+t+s)).$$

It follows that

$$-\sum_{j\in I_{r+1}}\sum_{l=r}^{k-j}b_l\sum_{t=5k-r-j-l}^{n}q^{n-t}\left(H(t-2k+j+l)-H'(t-2k+j+l)\right)$$

$$\leq \sum_{j\in I_{r+1}}\sum_{l=r}^{k-j}b_l\left(q^{n-5k+r+j+l+2}+(n-5k+r+j+l+1)q^{n-5k+j+l+r}\right)$$

$$+2(r-1)q^{n-5k+r+j+l+2}+2q^{n-7k+3s+j+l+r+1}\right)$$

$$\leq q^{n-3k-s+1}+q^{n-3k+r-s-2}+q^{n-3k+r-s-1}+q^{n-5k+2s+1}\leq q^{n-3k}.$$

$$(2.50)$$

One has

$$\sum_{j \in I_{r+1}} \sum_{l=r}^{k-j} b_l \sum_{t=4k-j-l}^{5k-r-j-l-1} q^{n-t} \delta(t-2k+j+l) \le 2 \sum_{j \in I_{r+1}} \sum_{l=1}^{k-j} b_l q^{n-5k+j+l+s+r}$$

$$\le 2(k-s-r-1)q^{n-4k+s+r+1} \le q^{n-3k}$$
(2.51)

and

$$\sum_{j \in I_{r+1}} \sum_{l=1}^{r-1} \sum_{t=3k+1}^{4k-j-l-1} q^{n-t} \tilde{b}'_{4k-t-j-l} \leq \sum_{j \in I_{r+1}} \sum_{l=1}^{r-1} \sum_{t=4k-s-j-l}^{4k-j-l-1} q^{n-t} b'_{4k-t-j-l}$$

$$\leq \sum_{j} \sum_{l=1}^{r-1} q^{n-4k+s+j+l+1} \leq \sum_{j \in I_{r+1}} q^{n-4k+s+j+r+1} \leq q^{n-4k+2s+r+2} \leq q^{n-3k+s}.$$
(2.52)

Finally, for  $3k - r \le n < 3k$ , using (2.43) and (2.49) one has the lower bound

$$\begin{aligned} \Delta(n) &\geq -2(q^{n-2k} + q^{n-4k+2s+r}) \\ &+ \sum_{t=3k-r}^{n} q^{n-t} \left( H(t-k+r) - \sum_{l=1}^{r-1} H'(t-k+l) - \sum_{l=r+1}^{s} b_l \delta(t-k+l) \right) \\ &\geq -2(q^{n-2k} + q^{n-4k+2s+r}) - \sum_{l=1}^{r-1} \sum_{t=3k-r}^{3k-l-1} q^{n-t} \tilde{b}'_{3k-t-l} - \sum_{l=r}^{s} \sum_{t=3k-r}^{n} b_l q^{n-t} \delta(t-k+l) \\ &\geq -2(q^{n-2k} + q^{n-4k+2s+r}) - \sum_{l=1}^{r-1} q^{n-3k+r+1} - 2\sum_{l=r}^{s} q^{n-4k+s+r+l} \\ &\geq -2(q^{n-2k} + q^{n-4k+2s+r}) - q^{n-3k+2r-1} - q^{n-4k+2s+r+2}. \end{aligned}$$

$$(2.53)$$

Applying (2.50) through (2.53) to (2.45), for  $4k - r \le n < 4k$  one thus has

$$\begin{split} &\Delta(n) \leq -q^{n-2k} + 2\sum_{t=3k+1}^{n} (q^{n-3k} + q^{n-5k+2s+r}) + \sum_{t=4k-r}^{n} (q^{n-4k+2r-1} + q^{n-5k+2s+r+2}) \\ &+ \sum_{t=3k+1}^{n} q^{n-t} H(t-k+r) + 2q^{n-3k} + q^{n-3k+s} \\ &\leq -q^{n-2k} + 2(k-1)(q^{n-3k} + q^{n-4k+s-2}) + (r-1)(q^{n-3k-5} + q^{n-4k+s}) \\ &+ (k-1)q^{n-3k+r} + 2q^{n-3k} + q^{n-3k+s} \\ &\leq q^{n-2k}(-1+q^{-2} + q^{-7} + q^{-11} + q^{-k-4} + q^{-1} + 2q^{-k} + q^{-3}) < 0 \end{split}$$

where we have used (2.38) and the inequalities  $k \ge 5$ ,  $(k-1) \le q^{k-3}$ , and  $k-1 \le q^{k/2}$ .

It follows that  $\tilde{\Delta}(n) < 0$  for n < 4k. In combination with our results from Section 6, one has

$$\Delta(n) < 0$$
 for  $n < 4k$  when  $s = s'$  and  $k = k'$ .

### 8. Numerical Results on Lengths of Short and Intermediate Time Intervals

If we think about the applicability of these results to finite time dynamics then one is led to the following key question: How long is the short time interval? Within this time interval it is possible to make finite time predictions of the dynamics. Another interval where such predictions can be made is the last (third) infinite time interval. Therefore it is of great importance in applications to estimate the lengths of two finite intervals, the short time interval where finite time predictions are possible and the second intermediate interval.

Clearly these lengths depend on k, i.e. the lengths of the words corresponding to the subsets of phase space (elements of the Markov partition) we consider. The short time interval starts at the moment n = k.

Theorem 3 gives a linear estimate of the length of the short time interval. However numerical simulations show that the lengths of both of these intervals grow exponentially (asymptotically as k increases) with the same base q, the number of symbols in the alphabet  $\Omega$  (i.e. number of elements in the Markov partition).

The following table presents the beginning and ending moments of the intermediate interval, i.e. the moment of time when the first and last pair of the first hitting probability curves intersect, respectively. Notably the length of the short time interval is always larger than the length of the intermediate interval. It appears that the ratio of lengths of these intervals converges in the limit when k tends to infinity

k	Beginning of interval	End of interval
4	20	26
5	37	52
6	70	103
7	135	208
8	264	415

Recall that as the number of elements in the Markov partition increases so too does k,

the length of the word representing each element. Therefore when we consider dynamics at finer scales, the length of the time interval on which predictions about the dynamics can be made seems to grow exponentially. Thus finite time predictions about the dynamics could be made on very long time scales if we consider a partition with a sufficiently large number of elements.

# 9. Concluding Remarks

Our results show that interesting and important finite time predictions for the dynamics of systems with the strongest chaotic properties and for the most random stochastic systems are possible. They also indicate how such predictions can be practically made. Numerical simulations [5] demonstrate that finite time predictions of some nonuniformly hyperbolic systems are also possible.

Although the theory of finite time dynamics of chaotic systems is completely in infancy, it is rather clear what to do next and which classes of dynamical systems these results should be generalized to. Some natural problems deal with words (elements of Markov partition) which have equal autocorrelations. One can also generalize our results for iid-like dynamical systems to those with nonuniform invariant measures and with non-equal transition probabilities. Work on these topics is in progress. A significant open problem is to develop relevant mathematical approaches and techniques, more dynamical than combinatorial in spirit, to handle new questions arising in studies of finite time dynamics.

# Acknowledgments

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#### **CHAPTER 3**

# **EXTENSION OF RESULTS ON PREDICTION OF ORBITS**

# 3.1 Introduction

In this chapter we briefly describe some natural generalizations of the theory appearing in Chapter 2, and describe some of the new difficulties that arise. As mentioned at the end of Chapter 2, each possible extension of the Theory presented there presents special difficulties. We describe these impediments here, at the same time proving some very basic results which will no doubt prove foundational for any relevant combinatorial arguments.

# 3.2 General Return Maps

One of the initial indications that a general theory like that in Chapter 2 might be possible came from numerical studies on the return map as it appears in billiards (an example of such a return map appears in Chapter 3, going by the name  $\mathcal{F}$ ). Consider an example in the form of the diamond billiard, whose sides are arcs of circles of different radii. We consider the

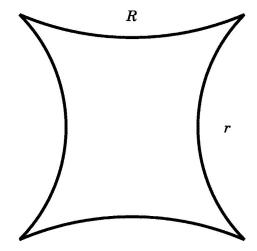


Figure 3.1: The diamond billiard

motion of a point particle as it moves inside the diamond. The particle travels in a straight

line until it reaches the boundary of the diamond. Upon collision with the boundary, the velocity vector of the particle changes according to the rule "the angle of incidence equals the angle of reflection," where the angle is measured relative to the tangent to the boundary. Obviously the motion is not defined when the particle strikes a corner point of the diamond, but such trajectories form a set of measure zero.

We can then define a "return map" on the boundary of the diamond. Let q be some point lying on the boundary of the diamond with direction v, ||v|| = 1, where v points inside the diamond. Let q' be the next point of the boundary that q hits as it moves in the direction v, and let v' be the direction after reflection off of the boundary at q'. Then  $\mathcal{F}(q, v) = (q', v')$ . In figure 3.2 we plot the first hitting probabilities of several subsets of the boundary.

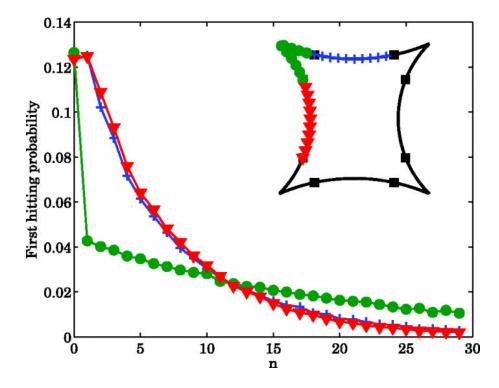


Figure 3.2: First hitting probabilities for various subsets of the diamond billiard

As one can see, these probabilities behave exactly as they do in Theorem 2. This is no coincidence. As it turns out, the trajectory of any point q with velocity v can be represented by a certain bi-infinite sequence  $\{b_i\}_{i=-\infty}^{\infty}$  where  $b_i \in \Omega$  and  $|\Omega| < \infty$ . In fact, any sequence  $\{b_i\}_{i=-\infty}^{\infty}$  with  $b_i \in \Omega$  is actually the representation of some trajectory. Calculating

the number of such sequences that first hit certain intervals on the boundary of the diamond billiard after n applications of  $\mathcal{F}$  reduces to counting the number of sequences of a finite length that avoid a certain pattern  $w_k \dots w_1$  everywhere, except that the sequence ends with  $w_k \dots w_1$ . This is exactly the context in which Theorems 1 and 2 apply.

More generally, similar return maps appear in other applications in physics. One typically has some map  $T : I \times \Omega \to \Omega$ , where I is a possibly infinite interval in time, that is rather complicated. In order to reduce the complication, one first picks some lower dimensional subspace of  $\Omega$ , call it P. Instead of considering the entire trajectory T(t, x) of some point  $x \in \Omega$ , one instead considers the sequence of points  $T(t_1, x), T(t_2, x), \ldots$  where  $t_i \in I$  are the moments in time t such that  $T(t, x) \in P$ .

In many interesting situations, the trajectory  $\{T(t_i, x)\}_{i=-\infty}^{\infty}$  can be encoded by a biinfinite sequence, as was possible in the case of the diamond billiard (and the Rössler system mentioned in the introduction). However, there is a catch. For the diamond billiard, any sequence  $\{b_i\}_{i=-\infty}^{\infty}$  with  $b_i \in \Omega$  was the representation of some trajectory. For general physical systems, not just any sequence is the representation of a trajectory. We are therefore interested, in general, in counting the number of strings that end with a given fixed word S, but which contain no instance of any member of some finite set of words  $\mathcal{A} = \{A, B, \dots, T\}$  with  $S \in \mathcal{A}$ . (This notation is adopted from [10]).

The time has come to at last introduce the general correlation function of two distinct words. This function, which is simply denote AB, is a binary string of length |A| where  $AB_i = 1$  if  $A_i \dots A_1 = B_{|B|} \dots B_{|B|-i+1}$ . For example, if A = HTHHTH and B =HTH, then AB = 000101. It will be helpful to write  $AB_x$  for the polynomial  $\sum_{i=1}^{|A|} b_i x^{i-1}$ . So, in our example,  $AB_x = 1 + x^2$ .

Denote the number of words which end with a fixed string S and avoid any member of  $\mathcal{A}$  (except possibly in the last |S| characters) by  $h_S(n)$ , and let a(n) denote the number of strings of length n that avoid any member of  $\mathcal{A}$ . Let  $F_S(x) = \sum_{i=1}^{\infty} h_S(i)x^i$  be the combinatorial generating function for  $h_S$ , and  $F(x) = \sum_{i=1}^{\infty} a(i)x^i$ . We call the set of words A reduced if I is never a subword of J for any I, J belonging to A. We will write |A| for the length of a word A. The authors [10] provide the following rather nice result regarding these generating functions:

**Theorem 3.2.1.** If  $\{A, B, ..., T\}$  is a reduced set of words, then the generating functions  $F(x), F_A(x), ..., F_T(x)$  satisfy the following system of linear equations:

$$(x-q)F(x) + xF_A(x) + xF_B(x) + \dots + xF_T(x) = x$$

$$F(x) - xAA_xF_A(x) - xBA_xF_B(x) - \dots - xTA_xF_T(x) = 0$$

$$\vdots$$

$$F(x) - xAT_xF_A(x) - xBT_xF_B(x) - \dots - xTT_xF_T(x) = 0$$
(3.1)

Denote

$$M = \begin{bmatrix} (x-q) & x & \dots & x \\ 1 & -xAA_x & \dots & -xTA_x \\ & \vdots & & \\ 1 & -xAT_x & \dots & -xTT_x \end{bmatrix}$$

and let

$$\phi(x) = \det(M).$$

It is observed in [10] that the matrix M is always invertible, and hence each generating function  $F_S(x)$  can be written as a rational polynomial with denominator  $\phi(x)$ . Therefore each function  $h_H(n)$  satisfies a recurrence with characteristic polynomial  $\phi(x)$ . Also shown in [10], presented there in the establishment of the system 3.1, are the following relations:

$$qa(n) = a(n+1) + h_A(n+1) + \dots + h_T(n+1)$$
  
$$a(n) = \sum_{i \in AS} h_A(n+i) + \sum_{i \in BS} h_B(n+i) + \dots + \sum_{i \in TS} b_T(n+i), \quad \forall H \in \mathcal{A}.$$
 (3.2)

In [10], relatively simple methods were employed to show that the largest root R of the characteristic polynomial of the recurrence a(n) is real. In [12], it was shown that R > R' if R' is the largest root of the characteristic polynomial of the recurrence a'(n).

Such estimates are much more difficult in the present context. The proof in [10] relies on the fact that the characteristic polynomial for a(n) can be written as (x - q)f(x) + 1where f(x) is a polynomial with coefficients equal to 0 or 1. This structure is completely lost in the determinant defining  $\phi(x)$ . In fact, as we will now demonstrate, one cannot hope for theorems quite as strong as those of chapter 2.

Let h(n) be the function obtained by solving the system of equations (3.1) with  $\mathcal{A} = \{w, A, B, \dots, T\}$ , and let h'(n) be the function obtained by solving the system with  $\mathcal{A} = \{w', A, B, \dots, T\}$ . Denote k = |w| and k' = |w'|. For the remainder of this section we let  $\mathcal{A} = \{A, B, \dots, T\}$ . We assume that  $\mathcal{A} \cup \{w\}$  and  $\mathcal{A} \cup \{w'\}$  are both reduced.

**Example 3.2.1.** Let  $\Omega = \{0, 1\}$  and  $\mathcal{A} = \{A, B\}$  where A = 10000 and B = 00000. Let w = 101 and w' = 011. Then h(n) - h'(n) < 0 for n < 11 and h(n) - h'(n) > 0 for  $n \ge 11$ . However the recurrence relation for h and h' is of order 13.

**Example 3.2.2.** Let  $\Omega = \{0, 1\}$  and  $\mathcal{A} = \{A, B\}$  where A = 1000 and B = 1111. Let w = 101 and w' = 011. Then cor(w) = 101 and cor(011) = 100, so that the hypothesis of Theorem 1 are satisfied. As one may check, the largest root in magnitude of  $\phi(x)$  is also the largest root in magnitude of  $\phi'(x)$ , and the root is real. In fact h(n) - h'(n) < 0 for large n.

We observe that the pathological behavior demonstrated in example 3.2.2 goes away as soon as A and B are "sufficiently large" relative to w.

**Example 3.2.3.** Let  $\Omega = \{0, 1\}$  and  $\mathcal{A} = \{A, B\}$  where A = 10000 and B = 11111. Let w = 101 and w' = 011. The largest roots of  $\phi(x)$  and  $\phi'(x)$  are real, and the largest root of  $\phi(x)$  is greater than the largest root of  $\phi'(x)$ .

**Proposition 3.2.1.** Let  $S \in A$  and  $\eta \ge |S|$ . Suppose that  $h_S(\eta) = 0$ . Then  $h_S(n) = 0$  for all  $n \ge \eta$ .

*Proof.* If x is any word counted by h(n) for some  $n > \eta$  then  $x_{\eta} \dots x_1$  is counted by  $h_S(\eta)$ , and there are no such strings.

In light of this proposition, we make the following definition: A set of words  $\mathcal{A}$  is called consistent if  $h_S(n) \neq 0$  for all  $n \geq |S|$  and  $S \in \mathcal{A}$ .

**Example 3.2.4.** Let  $\Omega = \{0, 1\}$  and  $\mathcal{A} = \{A, B\}$  where A = 100000 and B = 11111. Let w = 1010 and w' = 011. The largest roots of  $\phi(x)$  and  $\phi'(x)$  are both real, and the largest root of  $\phi(x)$  is greater than the largest root of  $\phi'(x)$ .

For any  $S, S' \in \mathcal{A}$  let  $H_{SS'}(n)$  denote the number of strings of length n that begin with S, end with S', and contain no other member of  $\mathcal{A}$ .

**Proposition 3.2.2.** Let  $S \in A$  and  $n \ge |S|$ . Then

$$qh_S(n) = h_S(n+1) + H_{AS}(n+1) + \dots + H_{TS}(n+1).$$

*Proof.* Let  $y = y_n \dots y_1$  be counted by  $h_S(n)$ . Consider the string  $y' = \omega y_n \dots y_1$  where  $\omega \in \Omega$ . This string is counted by exactly one of  $h_S(n+1), H_{AS}(n+1), \dots H_{TS}(n+1)$ . The result follows immediately.

The reason for the restriction  $n \ge |S|$  is that, as we saw in chapter 2, there may be some discrepancy between the function  $qh_S(n) - h_S(n+1)$  and the sum of functions  $H_{S'S}(n+1)$ . In particular, if n = |S| - 1, then  $h_S(n) = 0$ ,  $h_S(n+1) = 1$ , and thus at least one of the functions  $H_{S'S}(n+1)$  would have to be negative. We observe that the inequality  $H_{Sw}(n) \ge h(n - |S| - 1)$  holds for some choices of  $\mathcal{A}$ and w but not others. One may rewrite the statement of Proposition 3.2.2 as

$$h(n) = \sum_{S \in \tilde{\mathcal{A}}} H_{Sw(n)}$$

where  $\tilde{\mathcal{A}}$  is the set of sequences of length  $L = \max\{|S| : S \in \mathcal{A}\}$  that avoid any member of  $\{w\} \cup \mathcal{A}$ . This equality does two things: First, it gives us a means of actually calculating h(n) without explicit use of a recurrence relation (whose initial conditions we do not generally know). Second, it allows us to realize an explicit relationship between  $H_{Sw}(n)$  and h(n - L - 1) for any  $S \in \mathcal{A}$ . For any  $S \in \tilde{\mathcal{A}}$ , let  $\tilde{\mathcal{A}}_S = \{S' \in \tilde{\mathcal{A}} : S = \omega S'_L \dots S'_2$  for some  $\omega \in \Omega\}$ . Let us enumerate the members of  $\tilde{\mathcal{A}}$  as  $\{A_1, \dots, A_m\}$ , where  $m \leq a_w(L)$ .

One can imagine a graph  $\mathcal{G}$  where there is a directed edge going from vertex j to vertex i if  $A_j \in \tilde{\mathcal{A}}_{A_i}$ . Then the inequality  $H_{Sw}(n) \geq h(n - L - 1)$  surely holds if for each y counted by h(n - L - 1), there is an  $\omega \in \Omega$  such that the path of minimal length from  $A_j = \omega y_{n-L-1} \dots y_{n-2L+1}$  to  $A_i$  includes at least L vertices of  $\mathcal{G}$ . It is easy to create graphs where this does happen, such as when  $\mathcal{A} = \{1000, 0000\}$  and w = 101. It also easy to create graphs where this does not happen, such as when  $\mathcal{A} = \{1010, 0000\}$  and w = 111. In the former case, the inequality  $H_{Sw}(n) \geq h(n - L - 1)$  holds. In the latter case it does not.

The inequality  $H_{w'w'}(n) \ge h'(n-k'-1)$  was used in Chapter 2 to provide a greatly simplified proof for the case k > k'. Without such inequalities, a simple proof in the present context is currently unavailable. However, there are a few more simple statements that we can safely prove, and we do so now for the sake of posterity.

**Proposition 3.2.3.** Let  $S \in A$ . Then, for any  $\tilde{S} \in A$ , one has

$$h_{S}(n) = \sum_{S' \in \mathcal{A}} \sum_{i=1}^{|\tilde{S}|-1} \tilde{S}S'_{i}H_{S'S}(n+i) + H_{\tilde{S}S}(n+|\tilde{S}|).$$

Proof. Let  $y = y_n \dots y_1$  be any string counted by  $h_S(n)$ , and denote  $y' = \tilde{S}_m \dots \tilde{S}_1 y_n \dots y_1$ where  $\tilde{S} = \tilde{S}_m \dots \tilde{S}_1$ . Let *i* be the minimal index such that y' contains a member of  $\mathcal{A}$ beginning at position n + i, if there is such an *i*. If not, then y' is counted by  $H_{\tilde{S}S}(n)$ . Otherwise y' is counted by  $H_{S'S}(n+i)$  for some  $S' \in \mathcal{A}$ , and  $\tilde{S}S'_i = 1$  (here we denote the *i*-th entry of the binary sequence  $\tilde{S}S'$  as  $\tilde{S}S'_i$ , not to be confused with a polynomial in *i*). Conversely if  $\tilde{S}S'_i = 1$  then any string counted by  $H_{S'S}(n+i)$  arises from such a string y'. It follows that

$$h_{S}(n) = H_{\tilde{S}S}(n+|\tilde{S}|) + \sum_{i=1}^{m-1} \tilde{S}A_{i}H_{AS}(n+i) + \dots + \sum_{i=1}^{m-1} \tilde{S}T_{i}H_{TS}(n+i),$$

since  $\tilde{S}S'_{\tilde{S}} = 0$  for each  $S' \neq \tilde{S}$ , because  $\mathcal{A}$  is reduced.

**Corollary 3.2.2.**  $H_{Sw}(n) \leq h(n - |S|)$  for all  $S \in \mathcal{A}$  and  $n \geq |S| + 1$ .

Proof. According to Proposition 3.2.3 one has

$$h(n) = H_{Sw}(n+|S|) + \sum_{S' \in \mathcal{A}} \sum_{i=1}^{|S|-1} SS'_i H_{S'w}(n+i)$$
  

$$\geq H(n+|S|).$$

**Lemma 3.2.1.** Let k > k' and suppose that  $\mathcal{A} \cup \{w'\}$  is consistent. Then  $h(n) - q^{k-k'}h'(n-k+k') \le 0$  for  $n \le k+1$ .

*Proof.* Note that  $h(n) - q^{k-k'}h'(n-k+k') = 0$  for k-k' < n < k and  $h(n) - q^{k-k'}h'(n-k+k') = 1 - q^{k-k'} < 0$  when n = k. Let n = k+1 and  $0 \le m \le k-k'$ . Using Proposition 3.2.2 and the observation that  $H_{Sw}(k+1) \ge 0$  for all S, one has

$$h(k+1) - q^{m}h'(k'+1) = qh(k) - \sum_{S \in \mathcal{A}} H_{Sw}(k+1)$$

$$\begin{aligned} &-q^{m}\left(qh'(k') - \sum_{S \in \mathcal{A}} H_{Sw'}(k'+1)\right) \\ &\leq qh(k) - q^{m}\left(qh'(k') - \sum_{S \in \mathcal{A}} H_{Sw'}(k'+1)\right) \\ &= qh(k) - q^{m+1}h'(k') + q^{m}\sum_{S \in \mathcal{A}} H_{Sw'}(k'+1) \\ &\leq qh(k') - q^{m+1}h'(k') + (q-1)q^{m} \\ &\leq q^{m+1}(1 - h'(k')) \leq 0. \end{aligned}$$

The last inequality owes to the fact that  $\mathcal{A} \cup \{w'\}$  is assumed consistent. In the second to last inequality we have used the fact that at most (q-1) of the functions  $H_{Sw'}(k'+1)$  may equal 1, since  $\mathcal{A}$  is consistent. Let S be a string of greatest length such that  $H_{Sw'}(k'+1) = 1$ . Then  $Sw'_{|S|-1} = 1$ . Any other word S' such that  $H_{S'w'}(k'+1) = 1$  satisfies  $S_i = S'_{i-|S|+|S'|}$ for  $|S|-|S'|+1 \le i \le |S|-1$ . Since the set  $\mathcal{A} \cup \{w\}$  is reduced, it must be that  $S'_{|S'|} \ne S_{|S|}$ . There are obviously only q-1 choices for  $S'_{|S'|}$  that are distinct from  $S_{|S|}$ .

# 3.3 General Probability Distributions

We suppose now that we have a function  $p: \Omega \to [0, 1]$ , such that  $\sum_{\omega \in \Omega} p(\omega) = 1$ . Let V(n) denote the number of words of length n that end with w and which avoid it elsewhere. Denote by  $f(n) = \sum_{v \in V(n)} p(v)$ , the probability that a string  $v = v_n \dots v_1$  ends with w and  $v_{n-l+k} \dots v_{n-l+1} \neq w_k \dots w_1$  for  $k \leq l < n$ . Let F(n) = f(n-1) - f(n) and denote  $p(w) = \prod_{i=1}^{k} p(w_i)$  and  $w^{k-t} = w_{k-t} \dots w_1$ . The proof of the next lemma goes more or less exactly like the proof of Proposition 3.2.2, and is taken almost verbatim from [12], where we have replaced set cardinalities with probabilities.

## **Proposition 3.3.1.**

$$f(n) = f(n-1) - p(w)f(n-k) + \sum_{t=1}^{k-1} b_t p(w^{k-t})F(n-k+t).$$
 (3.3)

*Proof.* Let V be the set of words of length n that end with w and avoid it elsewhere, so  $|V| = h_w(n)$ . We partition V into subset  $V_i$ , each of size H(n + i) with i = 1, 2, ..., k, as follows. For any  $v \in V$  choose i to be the smallest index such that  $(wv)^i$  begins with w. If i < k, then clearly  $b_i = 1$ . Define  $V_i$  to be the set of all such v. Then  $V_i$  is in natural bijection with the set of all words of length n + i that begin and end with w, but avoid it elsewhere. This latter set can be constructed by taking all w-avoiding words of length n + i1, appending any of the q letters of  $\Omega$ , and then omitting all those words which are not counted by h(n + i). Thus one has

$$p(V_i) = f(n+i-1) - f(n+i),$$

and the recurrence follows.

Denote by  $g_h(x) = 1 + (x - q) \sum_{i=1}^k b_i x^{i-1}$  the characteristic polynomial of the recurrence  $g_h(n)$ . It is known, at least when q > 2, that the root of largest magnitude of C(x) is real and of multiplicity one [10]. The method of proof used Rouché's theorem, but the estimates and methods used there do not immediately generalize to the present context. We will prove a similar result (Theorem 3.3.2) using entirely different methods.

We denote by  $\mathcal{A}$  the set of all sequences of length k = |w| that avoid w. For  $A \in \mathcal{A}$ , denote by  $E_A(n)$  the set of all sequences of length n that begin with A, end with w, and avoid w elsewhere. Let  $f_A(n) = p(E_A(n))$ . Since the events  $E_A$  and  $E_B$  with  $A \neq B$  are disjoint and since every sequence counted by h(n) belongs to one of these events, we have

$$f(n) = \sum_{A \in \mathcal{A}} f_A(n).$$
(3.4)

Given  $\omega \in \Omega$ ,  $A = A_k \dots A_1$ , denote  $A_\omega = A_{k-1} \dots A_1 \omega$  and set  $A_\Omega = \{A_\omega : \omega \in \Omega\}$ . It is easy to see that  $E_A(n) = \sum_{A' \in A_\Omega} E_{A'}(n-1)$ , and again using the disjoint property of the sets  $E_{A'}$ , we have

$$f_A(n) = \sum_{A' \in A_\Omega} p(A_k) f_{A'}(n-1).$$
(3.5)

Let  $m = 2^k - 1$ , and note that  $|\mathcal{A}| = m$ . We will enumerate the elements of  $\mathcal{A}$  in an arbitrary fashion, and write  $\mathcal{A} = \{A_1, \ldots, A_m\}$ . Vectors in  $\mathbb{R}^m$  will be denoted with a bold script, for example  $\mathbf{v} \in \mathbb{R}^m$ , and the *i*-th entry of  $\mathbf{v}$  we will denoted by  $v_i$ . Let  $\boldsymbol{\sigma} \in \mathbb{R}^m$  be such that  $\sigma_i = 1, 1 \leq i \leq n$ , and let  $\mathbf{f}(n) \in \mathbb{R}^m$  be such that  $f_i(n) = f_{A_i}(n)$ . Relations (3.5) imply that there is some  $m \times m$  matrix T such that

$$\mathbf{f}(n) = T\mathbf{f}(n-1). \tag{3.6}$$

Relation (3.4) then shows that

$$f(n) = \boldsymbol{\sigma} \cdot \mathbf{f}(n) = \boldsymbol{\sigma} \cdot T\mathbf{f}(n-1) = \boldsymbol{\sigma} \cdot T^{n-k-1}\mathbf{f}(k+1).$$

This proves the following proposition.

# **Proposition 3.3.2.** $f(n) = \sigma \cdot T^{n-k-1} \mathbf{f}(k+1)$ .

We remark that if  $cor(w) \neq 2^k - 1$  then  $\mathbf{f}(k+1)$  has exactly q entries equal to 1, and all other entries are 0. If  $cor(w) = 2^k - 1$  then  $\mathbf{f}(k+1)$  has exactly q - 1 entries equal to 1, and all other entries are 0.

Let  $\overline{A}$  be the set of all words of length k, and let  $\overline{m} = 2^k$ . Let  $\overline{A} = {\overline{A}_1, \ldots, \overline{A}_{\overline{m}}} = {A_1, \ldots, A_m, w}$ . Recall that we denote the correlation of two words A and B by AB. Let M be the  $\overline{m} \times \overline{m}$  matrix whose (i, j)-entry, denoted  $M_{ij}$ , is given by

$$M_{ij} = \begin{cases} p((\overline{A}_i)_k) & \text{if } (\overline{A}_i \overline{A}_j)_{k-1} = 1 \\ 0 & \text{otherwise.} \end{cases}$$

It is easy to see that

$$T = M_{(\overline{m},\overline{m})}$$

where  $M_{(l,l)}$  denotes the submatrix of M obtained by removing row and column l.

**Lemma 3.3.1.** Let w be any word of length k such that s > 0. There exists a word E with |E| = k such that  $wE_i = 0$  for all i, and  $Ew_i = 0$  for all i.

*Proof.* Let  $\omega \in \Omega$  be such that  $\omega \neq w_k$ . Observe that  $C = \omega \dots \omega$ , |C| = k, has the property that  $wC_i = 0$  for all *i*. Similarly let  $\omega \in \Omega$  be such that  $\omega \neq w_1$ . The word  $D = \omega \dots \omega$  has the property that  $Dw_i = 0$  for all *i*. Moreover, if  $b_1 = 1$  then  $w_k = w_1$  and the word  $\omega \dots \omega$  works for both *C* and *D*, where  $\omega \neq w_k$  is arbitrary. Hence E = C = D in this case. It therefore suffices to assume that  $b_1 = 0$ .

Let  $t = \max\{\ell \ge 0 : \exists i \text{ such that } w_{i-j+1} = w_k \forall 1 \le j \le \ell\}$ . The number t is the length of the longest string of consecutive characters  $w_k$  that appears in w. If t = k then  $b_1 = 1$ . Otherwise let  $C = w_k \dots w_k$  have length t + 1 and  $D = \omega \dots \omega$  have length k - t - 1. We claim that E = C \* D has the desired property.

We demonstrate first that  $wE_i = 0$  for all *i*. Clearly  $wE_i = 0$  for i > t+1, since *w* does not contain  $E_k \dots E_{k-t}$ . The fact that  $wE_i = 0$  for  $i \le t+1$  follows from the assumption that  $b_1 = 0$ , whence  $w_1 \ne w_k$  and  $wE_i = 1$  implies  $w_1 = w_k$ .

We now show that  $Ew_i = 0$  for all *i*.

Observe that  $Ew_i = 0$  for all i < k - t and for i = k. Suppose  $Ew_i = 1$  for some  $k - t \le i < k - 1$ . One has  $w_k \dots w_{k-\delta+1} = w_k \dots w_k$  where  $\delta = i - (k - t) + 1$ , and  $w_{k-\delta} \dots w_{k-i+1} = \omega \dots \omega$ . Observe that  $\delta < t$ . This forces  $w_{k-i} \dots w_1$  to contain t consecutive characters equal to  $w_k$ . This is a contradiction as, by assumption, k - i < t. If i = k - 1 then the assumption s > 0 implies that  $b_j = 1$  for some  $j \le k - t$ . Since  $w_l = \omega$  for  $2 \le l \le k - t$  and  $b_1 = 0$ , this is a contradiction.

We remark that the word E constructed in Lemma 3.3.1 does not have the desired properties when s = 0. Consider as a counter example w = 100 over the alphabet  $\Omega = \{0, 1\}$ . Then E = 110 and  $Ew_2 = 1$ .

**Corollary 3.3.1.** Let w be such that s > 0. The matrix T is irreducible and aperiodic.

*Proof.* Let  $A_i \in \mathcal{A}$  and  $A_j \in \mathcal{A}$  be arbitrary. Using the sequence E described in Lemma 3.3.1, clearly  $A_j * E * A_i$  does not contain a copy of w. It follows that  $T_{i,j}^{2k-1} \ge p(A_j * E) > 0$ .

To see that T is aperiodic, let  $\omega \neq w_k$ . The word  $A_j = \omega \dots \omega$  is in  $\mathcal{A}$ . Since  $\omega(A_j)_k \dots (A_j)_2 = A$ , one has  $T_{jj} \geq p(\omega) > 0$ .

Applying the Perron-Frobenius theorem to T, we conclude that there is a real eigenvalue r of T satisfying

$$|r| > \max\{|\lambda| : \lambda \neq r \text{ is an eigenvalue of } T\}.$$

Using Proposition 3.3.2 we have

$$\frac{1}{r^{n-k-1}}f(n) = \boldsymbol{\sigma} \cdot \frac{1}{r^{n-k-1}}T^{n-k-1}\mathbf{f}(k+1)$$
$$\to \boldsymbol{\sigma} \cdot P\mathbf{f}(k+1),$$

where P is the matrix of the projection onto the eigenspace of r. Since the projection P is known to be a positive matrix and since f(k + 1) is a 0 - 1 vector, Pf(k + 1) = cv where c is a positive constant. Thus

$$\frac{1}{r^{n-k-1}}f(n) \to c\boldsymbol{\sigma} \cdot \mathbf{v}.$$
(3.7)

Proposition 3.3.2 implies that

$$\boldsymbol{\sigma} \cdot g(T)T^{n-d(g)-k-1}\mathbf{f}(k+1) = 0$$

for all  $n \ge d(g) + k + 1$ , where d(g) is the degree of g(x). It follows that

$$\boldsymbol{\sigma} \cdot g(T) \frac{1}{r^{n-d(g)-k-1}} T^{n-d(g)-k-1} \mathbf{f}(k+1) = 0$$

for all such n as well. As discussed,  $\frac{1}{r^{n-d(g)-k-1}}T^{n-d(g)-k-1}\mathbf{f}(k+1)$  tends to  $c\mathbf{v}$  for some c > 0. One then has

$$\boldsymbol{\sigma} \cdot g(T) \frac{1}{r^{n-d(g)-k-1}} T^{n-d(g)-k-1} \mathbf{f}(k+1) \to c \boldsymbol{\sigma} \cdot g(T) \mathbf{v}$$

Observe that

$$\boldsymbol{\sigma} \cdot g(T)\mathbf{v} = \boldsymbol{\sigma} \cdot g(r)\mathbf{v} = g(r)\boldsymbol{\sigma} \cdot \mathbf{v}.$$

Since  $\boldsymbol{\sigma} \cdot \mathbf{v} \neq 0$ , the limit

$$cg(r)\boldsymbol{\sigma} \cdot \mathbf{v} = \lim_{n} \boldsymbol{\sigma} \cdot g(T) \frac{1}{r^{n-d(g)-k-1}} T^{n-d(g)-k-1} \mathbf{f}(k+1) = 0$$

implies that g(r) = 0. All together these remarks prove the following theorem:

**Theorem 3.3.2.** Let w be such that s > 0. Let r denote the largest positive eigenvalue of the matrix T. Then g(r) = 0 and

$$\lim_{n \to \infty} \frac{f(n)}{r^n} = c$$

for some c > 0.

Examples indicate that much stronger results may be true.

**Conjecture.** Let w be such that s > 0. Then g(T) = 0, and r is the largest real root of g(x).

## **CHAPTER 4**

# PHYSICAL BILLIARDS AND EHRENFESTS' WIND-TREE MODEL

# Introduction

It is a commonly held opinion that mathematical billiards generated by the motion of a point particle adequately describes the dynamics of real physical particles within the same domain (billiard table). We show here that this opinion is wrong for billiards in non-convex polygons. The same is true for billiards in non-convex polyhedrons. Namely, it is well known that billiards in polygons and polyhedrons are non-chaotic and have zero Kolmogorov-Sinai entropy [13, 14]. We show here that on the contrary physical billiards in non-convex polygons are hyperbolic. Therefore such billiards are chaotic and have positive Kolmogorov-Sinai entropy. Formally we prove hyperbolicity of billiards in rational non-convex polygons extremely well approximated by rational polygons. However, there is no doubt that physical billiards in general non-convex polygons are also chaotic (hyperbolic).

Then we apply these results to the classical Ehrenfests' Wind-Tree model [7]. This model has been studied extensively by physicists [15, 16, 17, 18, 19, 20]. In this model a point particle (Wind) moves by inertia in an array of immovable (infinitely heavy) scatterers which have the shape of rhombuses (Trees). Upon reaching the boundary of a Tree the particle (Wind) gets reflected elastically. The Wind-Tree model was introduced by the Ehrenfests as a simple model of diffusion. It was shown however that the Wind-Tree model is non-chaotic (in particular it has zero Kolmogorov-Sinai entropy) and therefore the Wind-particle does not move diffusively.

Instead the Lorentz gas, where the scatterers are circles, became a classical and very

popular "simplest" mechanical model of diffusion. We rehabilitate here the Ehrenfests' Wind-Tree model as a simple model of diffusion by taking the Wind to be a real physical particle, i.e. a particle with a finite (non-zero) size. Moreover, we show that the Wind-Tree model with a physical (disk) particle is at least as dynamically rich as the Lorentz gas.

This last point means that the physical Wind-Tree particle has at least as many different dynamical regimes as the Lorentz gas does. In particular the Wind-Tree model may have a finite as well as an infinite horizon (i.e. bounded or unbounded free path). Also, a very natural and beautiful variant of the Wind-Tree model arises if one considers trees in the shape of two different rhombuses as in the famous R. Penrose tiling [21]. Then we get a quasi-crystal Wind-Tree model where the dynamics is also hyperbolic. Other modifications to the classical Wind-Tree model have been suggested with the goal of making it more dynamically rich [22, 23, 24]. Our observation is that it suffices to consider a physical particle instead of a point particle.

The free motion of a circular particle interior to a polygon **D** will be considered. We will always assume that the speed of the particle is 1. If the point particle does not collide with the boundary  $\partial$ **D** at any moment in time up to *t*, then its motion is governed by the equations

$$\dot{q} = v$$
$$\dot{v} = 0.$$

If it does collide with the boundary (and not at a corner) at some moment in time  $0 < s \leq t$ , then at the moment of collision its velocity changes according to the rule 'the angle of reflection equals the angle of incidence.' That is, its direction after collision is  $v - 2(v \cdot n)n$ , where n is the inner unit normal vector with respect to  $\partial \mathbf{D}$ . In the following section we will formally describe the motion of a physical particle.

#### 4.1 Preliminaries

Let **D** be a polygon in  $\mathbb{R}^2$ . We will write  $\partial \mathbf{D} = \bigcup_j \Gamma_j$ , where each each  $\Gamma_j$  is given by a function  $f_j : [0,1] \to \mathbb{R}^2$  whose image is a line segment. We assume that the boundary components can intersect each other only at their endpoints, that is

$$\Gamma_i \cap \Gamma_j \subset \partial \Gamma_i \cup \partial \Gamma_j.$$

Moreover, we assume that  $\Gamma_i \cap \Gamma_j$  is either empty or a single point. We will refer to any point belong to  $\bigcup_{i \neq j} \Gamma_i \cap \Gamma_j$  as a corner point.

Let r be any fixed positive number. Denote by D the set  $\mathbf{D} \cap \{x : d(x, \mathbf{D}) \geq r\}$ . We remark that the definitions in this and the following paragraph apply equally well if we replace D with D. Consider the set  $\Omega = \Omega(D) = D \times S$ , where S is the unit circle. If  $q \in \partial D$  is not a corner point, then let  $n_q$  be the inner unit normal vector with respect to the boundary at q. Denote the tangent space of  $\Omega$  by  $T\Omega$  and let  $w, w' \in T\Omega$ . For  $x = (q, v) \in \Omega$  with  $q \in \partial D$  we identify the tangent vectors w and w' which satisfy the equality  $w' = w - 2(w \cdot n_q)n_q$ , and denote the resulting quotient of the tangent space as  $\mathcal{T}$ . We will denote the members of  $\mathcal{T}$  by  $\hat{w}$  for  $w \in T\Omega$ .

The space  $\mathcal{T}$  of course no longer coincides with  $T\Omega$ , but we can nonetheless refer to functions  $v: \Omega \to \mathcal{T}$  as vector fields. We say that  $\Phi(x,t)$  is a flow if  $\widehat{\frac{d}{dt}\Phi(x,t)} = v(x)$  at every  $x = (q, v) \in \Omega - \partial D \times S^1$ , and if the one-sided derivatives of  $\Phi(x, t)$  exist and equal v(x) (in the sense of  $\mathcal{T}$ ) at every  $x \in \partial D \times S^1$ .

The specific vector field which represents the motion of a particle reflecting as described in the introduction is given by w(x) = w(q, v) = v, and we refer to its flow  $\Phi(x, t)$  as a billiard flow. Whenever we speak of a "physical billiard," we are referring to the billiard flow  $\Phi$ . Observe that  $\Phi(x, t)$  is not defined for any t > 0 when q is a corner point and x = (q, v).

Let  $\tilde{\Omega} = \tilde{\Omega}(D)$  be the subset of  $\Omega$  on which  $\Phi$  is defined for all  $t \ge 0$ . We will refer to

the members of  $\hat{\Omega}$  as regular points. It is a well known fact that almost every point of  $\Omega$  is a regular point.

In the following two propositions we will assume that if  $\Gamma_i$  and  $\Gamma_j$  are two components of the boundary such that  $\Gamma_i \cap \Gamma_j = \emptyset$ , then the distance between them is greater than r. This assumption is not necessary, however. The results proved in Section 2 will continue to hold as long as there is at least one corner point p with interior angle greater than  $\pi$  that the circular particle is able to hit.

**Proposition 4.1.1.** Let  $c = \Gamma_i \cap \Gamma_j$  be a corner point. Suppose that the angle  $\angle \Gamma_i \Gamma_j$ measured interior to **D** is greater than  $\pi$ . Then there is a neighborhood of *D* in which  $\partial D$ is a circular arc.

*Proof.* Let  $R = \min\{d(c, \Gamma_k) : k \neq i, j\}$ . Note that R > r by assumption. Denote by B the ball of radius R centered at c, let  $n_i$  be the inner unit normal to  $\Gamma_i$ , and let  $n_j$  be the inner unit normal to  $\Gamma_j$ . By assumption,  $\Gamma_k \cap B = \emptyset$  for  $k \neq i, j$ . It follows that  $\partial D \cap B$  is the union of  $(\Gamma_i + n_i) \cap B$  and  $(\Gamma_j + n_j) \cap B$  together with the circular arc connecting  $c + n_i$  to  $c + n_j$ . For any point q in the circular arc, there is a small ball b centered at q such that  $\partial D \cap b$  is an arc of a circle.

Figure 4.1 can be taken as an illustration of the situation in general, which is summarized in Proposition 2.4.2.

**Proposition 4.1.2.**  $\partial D = \bigcup_j \Gamma_j$  where each  $\Gamma_j$  has constant curvature equal to either 0 or  $k = \frac{1}{r}$ .

Let  $\mathcal{P}$  be the set of polygonal domains in  $\mathbb{R}^2$ . For any  $\mathbf{P} \in \mathcal{P}$ , we will refer to the flow  $\Phi$  defined on  $\Omega(P)$  as a physical billiard. Let  $\mathcal{P}_n \subset \mathcal{P}$  be the collection of domains whose boundaries have n vertices. Denote by  $\mathcal{R}$  the collection of domains whose boundaries have angles which are rational multiples of  $\pi$ , and denote by  $\mathcal{R}_n \subset \mathcal{R}$  the subset whose boundaries have n vertices.

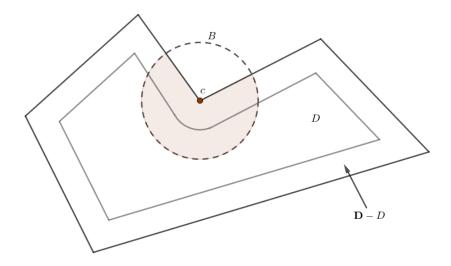


Figure 4.1: The corner c together with the ball B.

Let  $S_P$  denote the set of points of  $\partial P$  at which the curvature of  $\partial P$  does not exist. Such points can be characterized as corners of the boundary of P and intersections between linear components and components which are circular arcs. We denote by  $C_P$  the set of connected components of  $\partial P - S_P$ . For  $x \in \partial P$  denote by  $\kappa_P(x)$  the curvature of  $\partial P$  at x, when it exists. We observe that the curvature takes on one of two possible values, namely 0 or  $k = \frac{1}{r}$ . One has  $C_P = C_P^f \cup C_P^k$  where  $C_P^f$  is the set of components which have zero curvature and  $C_P^k$  is the set of components which have curvature k.

The set  $\mathcal{P}_n$  can be identified with  $\mathbb{R}^{2n-2}$ , and this space is complete with respect to the usual Euclidean metric [25]. To make the identification, we think of  $P \in \mathcal{P}_n$  as being determined by its boundary. The boundary can be identified with a polygon having one vertex fixed at the origin, and so  $\partial \mathbf{P}$  is specified entirely by the coordinates of its other n-1 vertices.

Let  $\mathcal{O} \subset \mathcal{P}$  be the set of tables which have at least one angle greater than  $\pi$ . Note that  $\mathcal{O}$  is open in the topology of  $\mathbb{R}^{2n-2}$ . Denote by  $\mathcal{O}_n^m \subset \mathcal{O} \cap \mathcal{P}_n$  the collection of polygons  $\mathbf{P}$  which have a dense set of orbits that hit  $C_P^k$  at least m times. For any fixed t > 0 the function  $\Phi$  depends continuously both on x and the parameters of the table viewed as a

point in  $\mathbb{R}^{2n-2}$ . As a result, the set  $\mathcal{O}_n^m$  is open in  $\mathcal{P}_n$ .

Theorem 4.2.3 shows that every rational polygon table in  $\mathcal{O}$  is a member of  $\mathcal{O}_n^m$ . Thus the sets  $\mathcal{O}_n^m$  are dense, and the collection  $G_n = \bigcap_{m=1}^{\infty} \mathcal{O}_n^m$  is a dense  $G_{\delta}$  subset of  $\mathcal{R}_n$ . Let  $\mathcal{G} = \bigcup_n G_n$ . We say that D (or **D**) is generic if D belongs to a dense  $G_{\delta}$  subset of  $\mathcal{O}$ .

A flow  $\Phi$  on a domain D (or **D**) is topologically transitive if for almost every  $x \in \tilde{\Omega}$  the sets  $\{\Phi(x,t)\}_{t=0}^{\infty}$  and  $\{\Phi(x,t)\}_{t=-\infty}^{0}$  are dense in D (or **D**).

## 4.2 Generic Physical Billiards are Topologically Transitive

We begin by summarizing the main result of [25].

**Theorem 4.2.1.** There is an everywhere dense subset of  $\mathbb{R}^{2n-2}$  of type  $G_{\delta}$  such each polygon with vertices in this set has billiard flow  $\Phi$  which is topologically transitive.

Throughout the rest of this section we will denote  $\Phi((q, v), t) = (q_t, v_t)$ . By an abuse of notation, we will write  $q \in C_D^k$  if  $q \in \bigcup_{\Gamma \in C_D^k} \Gamma$ .

**Corollary 4.2.2.** Suppose that  $q_{\tau} \in C_D^k$  and let  $\epsilon > 0$  be arbitrary. There exists an open set  $U \subset \Omega(D)$  with  $x \in U$  and t with  $|t - \tau| < \epsilon$  such that each point  $(p, w) \in U$  will satisfy  $p_t \in C_D^r$  with  $w_t$  not tangent to  $\partial D$ .

*Proof.* Denote x = (q, v), and let  $\Gamma \in C_D^k$  be such that  $q_\tau \in \Gamma$ . Let L be the straight line segment that connects the boundary points  $b_1$ ,  $b_2$  of  $\Gamma$ . Let  $a \neq x$  be a point in D such that the triangle  $\Delta$  formed by the line segments  $\overline{ab_1}$ ,  $\overline{b_1b_2}$ , and  $\overline{b_2a}$  contains x, and such that  $\Delta \cap D$  is connected. By  $Y \subset S^1$  we denote the collection of unit vectors u which are parallel to  $t(b_1 - a) + (1 - t)(b_2 - a)$  for some 0 < t < 1.

It is easy to extend the vector field v to all of  $\Delta \times S^1$ ; if  $v_{(p,w)} = w$  for  $(p,w) \in \Omega$ , then let  $\tilde{v}_{(p,w)} = w$  for  $p \in \Delta$ . Let  $\tilde{\Phi}$  be the flow corresponding to  $\tilde{v}$ . It is easy to see that  $\tilde{\Phi}$ carries (p,w) to (p',w') where  $p' \in L$ . Since  $\tilde{\Phi} = \Phi$  for every t such that  $q_t \in D$ , the flow  $\Phi$  carries each point of  $\Delta \times Y$  into  $C_D^k$ . The set  $\Delta \times Y$  is open in the subspace topology of D. It is a well known fact that the flow  $\Phi(x,t)$  is continuous in x for each fixed t. Therefore  $U = \Phi^{-1}(\Delta \times Y, \tau)$  is open in  $\Omega$ , and each point  $(p, w) \in U$  hits  $C_D^k$  at some moment in time t > 0. Note that U is non-empty. Moreover by replacing  $\Delta$  with a sufficiently small ball around  $q_{\tau}$ , it is possible to ensure that the impact time t of any point  $(p, w) \in W \times X$  satisfies  $|t - \tau| < \epsilon$ . Similarly, by making Y sufficiently restricted we may assume that w is not tangent to  $\Gamma$ .

The following theorem is the main result of this section. Whenever we say that a trajectory has struck or hit a component  $\Gamma$  of the boundary, what we mean is that  $q_t \in \Gamma$  and  $v_t$  is not tangent to  $\Gamma$ .

**Theorem 4.2.3.** Let **D** be generic. There is a dense set of points  $x \in \Omega$  for which the corresponding physical billiard hits vertices with angle greater than  $\pi$  infinitely many times.

*Proof.* For any  $\mathbf{D} \in \mathcal{R}$  we can find a table  $\mathbf{R} \in \mathcal{R}$  such that  $D \subset \mathbf{R}$  and  $C_D^f \subset C_{\mathbf{R}}^f$ . We can also choose  $\mathbf{R}$  so that each component of  $\mathbf{R} - D$  is convex, as illustrated in figure 4.2.

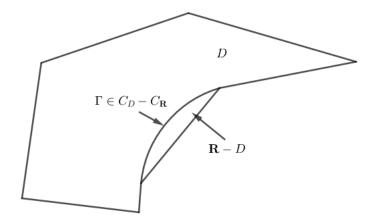


Figure 4.2: Domains D and  $\mathbf{R}$ .

Let  $V = \mathbf{R}^{\circ} - B$  and U be an open subset of  $\Omega(D)^{\circ}$ . The set U is also open in  $\Omega(\mathbf{R})$ . There is a point  $x = (q, v) \in U$  such that  $\bigcup_{t=0}^{\infty} q_{\mathbf{R},t}$  is dense in  $\mathbf{R}$ , where  $\Phi_{\mathbf{R}}(q, v) = (q_{\mathbf{R},t}, v_{\mathbf{R},t})$  is the flow with respect to  $\mathbf{R}$ . Since V is open in  $\mathbf{R}$  there exists t such that  $q_{\mathbf{R},t} \in V$ , and thus there is a minimal  $t' \geq 0$  such that  $q_{\mathbf{R},t'} \in \partial V$  and  $v_{\mathbf{R},t'}$  is not tangent to V. One has  $\Phi(x,t) = \Phi_{\mathbf{R}}(x,t)$  for  $0 < t \le t'$ , and so  $q_{t'} \in \partial V$ . Therefore  $q_{t'} \in C_D^k$ . Using Corollary 4.2.2, there is an open set  $U_1 \subset \Omega(D)$  and a moment of time  $\tau_1$  such that for each  $y = (p,w) \in U_1$  one has  $p_t \in C_D^k$  for some t satisfying  $|t - \tau_1| < \epsilon$ .

We assume that there exists a sequence of sets  $U_i$  and times  $\tau_i$  for  $1 \le i \le n-1$  such that  $U_i \subset U_{i-1}$  and for every  $x \in U_i$  there exists a sequence  $t_j$  such that  $x_{t_j} \in C_D^k$  for  $1 \le j \le i$  where  $|t_j - \tau_j| < \epsilon$ .

The image  $\Phi(U_{n-1}, \tau_{n-1} + 2\epsilon)$  contains an open set, which we denote  $U'_{n-1}$ . Since the map  $\Phi(x, t)$  is continuous for finite t, the pre-image  $\Phi(U'_{n-1}, \tau_{n-1} + 2\epsilon)^{-1}$  is open in  $\Omega$  and is a subset of  $U_{n-1}$ . Since  $U'_{n-1}$  can be assumed to be an open subset of  $\Omega(\mathbf{R}) - V \times S^1$ , there is a point  $y = (p, w) \in U'_{n-1}$  with a dense trajectory under  $\Phi_{\mathbf{R}}$ . If  $x' = (q', v') = \Phi^{-1}(y)$ , then  $x' \in U_{n-1}$  and there is some  $t_{n-1}$  for which  $\Phi(x', t_{n-1}) \in C_D^k$ . Since the trajectory of y is dense under  $\Phi_{\mathbf{R}}$ , there exists a minimal moment of time s such that  $p_{\mathbf{R},s} \in C_D^k$  and  $w_{\mathbf{R},s}$  is not tangent to  $\partial V$ , where  $\Phi_{\mathbf{R}}(y, s) = (p_{\mathbf{R},s}, w_{\mathbf{R},s})$ . We denote  $\tau_n = s + t_{n-1} + 2\epsilon$ , and observe that  $\tau_n \geq \tau_{n-1} + 2\epsilon > t_{n-1}$ .

By definition  $\Phi(x', \tau_{n-1} + 2\epsilon) = y$ . For  $t_{n-1} + 2\epsilon \leq t \leq t_n$  one has  $\Phi(x', t) = \Phi(y, t - \tau_{n-1} - 2\epsilon) = \Phi_{\mathbf{R}}(y, t - \tau_{n-1} - 2\epsilon)$ , and therefore  $\Phi(x', \tau_n) \in C_D^k$  and  $v'_{\tau_n}$  is not tangent to  $\partial D$ . Again applying Corollary 4.2.2, there is an open set  $U_n \subset U_{n-1}$  such that for each  $\tilde{x} = (\tilde{q}, \tilde{v}) \in U_n$  one has  $\tilde{q}_t \in C_D^k$  for some t satisfying  $|t - \tau_n| < \epsilon$ , and  $\tilde{v}_t$  is not tangent to  $\partial D$ .

One can choose the sets  $U_i$  so that  $U_{i+1} \subset \overline{U_{i+1}} \subset U_i$ . We may therefore assume that the sets  $U_i$  are closed. Their intersection is therefore non-empty, and any point x = (q, v)contained in their intersection belongs to each of the sets  $U_i$ . The point x = (q, v) therefore strikes  $C_D^k$  infinitely many times. Since this construction is independent of the choice of open set U, the set of all points x that strike  $C_D^k$  infinitely many times is dense in  $\Omega(D)$ .  $\Box$ 

# 4.3 Hyperbolicity of generic physical billiards

A summary of the results in this section can be found in [26], among many other sources. Let  $\mathcal{M} = \bigcup_i \mathcal{M}_i$  where  $\mathcal{M}_i = \{x = (q, v) \in \Omega : q \in \Gamma_i, v \cdot n \ge 0\}$ . For each regular point x, there exists a  $\tau(x) > 0$  such that  $\Phi(x, \tau) \in \mathcal{M}$ . For each  $x \in \mathcal{M} \cap \Omega(D) = \tilde{\mathcal{M}}$  one may then define the following map from  $\tilde{\mathcal{M}}$  to itself:

$$\mathcal{F}(x) = \Phi(x, \tau(x)).$$

There exists a  $\mathcal{F}$ -invariant set  $H \subset \tilde{\mathcal{M}}$  with  $\mu(H) = 1$  such that for all  $x \in H$  there is a  $D\mathcal{F}$ -invariant decomposition of the tangent space

$$T_x M = E_x^1 \oplus E_x^2.$$

(See [26]). For each nonzero vector  $v \in E_x^i$ , one has

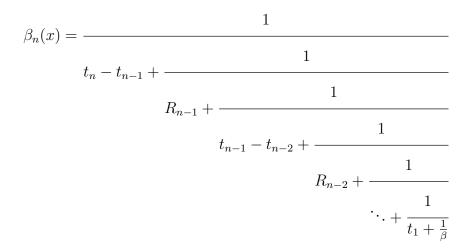
$$\lim_{n \to \pm \infty} \frac{1}{n} ||D_x \mathcal{F}^n v|| = \lambda_x^i,$$

with  $\lambda_x^1 > \lambda_x^2$ .

The numbers  $\lambda_x^i$  are called Lyapunov exponents of the map  $\mathcal{F}$  at the point x. A point x is said to be hyperbolic if Lyapunov exponents exist at x and none of them equals zero. The map  $\mathcal{F}$  is said to be hyperbolic if almost every point x of its domain is hyperbolic.

For any regular point x, let  $\{t_j\}_{j=1}^{\infty}$  be the collection of times during which  $q_{t_i} \in \partial D$ .

Denote by  $\kappa_j$  the curvature of  $\partial D$  at the point  $q_{t_i}$ , and define



where

$$R_i = \frac{2\kappa_i}{\cos(\phi_i)},$$

 $\beta$  is a constant, and  $\phi_i$  is the angle between  $v_{t_i}$  and the inner unit normal to the boundary.

According to the Seidel-Stern theorem (found e.g. in [27]), a necessary and sufficient condition for convergence of the sequence  $\beta_n(x)$  is that

$$\sum |t_n - t_{n-1}| + \sum |R_{n-1}| = \infty.$$
(4.1)

According to Theorem 4.2.3, if D is generic then for almost every  $x \in \tilde{\Omega}$  there is a sequence  $\{\tau_i\}_{i=1}^{\infty}$  such that  $q_{\tau_i} \in C_D^k$ . There is a subsequence  $j_i$  such that  $t_{j_i} = \tau_i$ . One has  $\kappa_{j_i} = k$  and  $\kappa_j = 0$  for  $j \notin \{j_i\}_{i=1}^{\infty}$ . Then  $|R_{j_i}| = |\frac{2k}{\cos(\phi_i)}| \ge 2k$  for infinitely many i, and thus the relation (4.1) is satisfied. Note that  $\lim_n \beta_n(x) > 0$ .

One has the following formula for the Lyapunov exponent  $\lambda_x^1$ :

$$\lambda_x^1 = \lim_{t \to \infty} \frac{1}{t} \log \prod_{i=0}^n |1 + s_i \beta_i|$$

where  $s_0 = t_1$ ,  $s_i = t_{i+1} - t_i$  for  $1 \le i \le n-1$ , and  $s_n = t - t_n$ . From the convergence of the sequence  $\beta_n$ , it follows immediately that  $\lambda_x^1 > 0$ . Additionally, the Lyapunov exponents sum to zero almost everywhere because billiards are Hamiltonian systems:

$$\lambda_r^1 + \lambda_r^2 = 0$$

As a result, the map  $\mathcal{F}$  is hyperbolic and therefore a chaotic dynamical system.

## 4.4 Ehrenfests' Wind-Tree Model

The following discussion largely mirrors that of [25]. We consider now a domain D which is a subset of the 2-dimensional torus  $T^2$  with Euclidean metric. This domain D is obtained from  $T^2$  by removal of a single rhombus, and we assume that the angle between any adjacent sides of the rhombus is a rational multiple of  $\pi$ . In particular, we define  $T^2$  to be the unit square of  $\mathbb{R}^2$  centered at zero with the usual identification of sides. The domain Dresults by subtracting from the unit square a rhombus, which we assume does not intersect the boundary of the square, and then identifying the sides of the square. We consider the flow  $\Phi(x, t) : \Omega_D \to \Omega_D$  defined as before.

The following remarks are largely elementary, but since they are frequently omitted from exposition on the subject we will elaborate somewhat for the sake of clarity.

Fix a direction e parallel to one side of the rhombus. If a vector v makes angle  $\phi$  relative to e, then the identification of the vectors v and  $v - 2(v \cdot n(q))n(q)$  at points q on the boundary of D then identifies  $\phi$  with  $2\alpha - \phi$ . Denote by  $\tau_i$  the impact times of  $q_t$  with  $\partial D$ . Let the tangent to the boundary of D make angle  $\delta_i$  with e. Denote

$$\phi_i = 2\delta_i - \phi_{i-1}$$

where  $\phi_i$  are the angles made by  $v_{\tau_i}$  with e. It is easy to see that

$$\phi_i \in \left\{ j \frac{m}{n} \pi \pm \phi \right\}_{j=0}^{2n-1} = \mathcal{A}$$

for every *i* and any  $\phi$ .

Consider the subset  $D(\phi) = D \times v(\phi) \subset D \times S^1$ . Clearly  $\bigcup_{t=-\infty}^{\infty} \Phi(x,t) \subset \bigcup_{\phi \in \mathcal{A}} D(\phi) = W$ . Generally  $|\mathcal{A}| = 2n$ , so we will denote  $W = \bigcup_{i=1}^{2n} D(\psi_i)$ . Denote  $U = \bigsqcup_{i=1}^{2n} D(\psi_i)$  and points in U by (q, i). We introduce the following collection M of subsets of U, as follows: It consists of all the one point sets (q, i) where  $q \notin \partial D$ , and the following types of two-point sets:

$$\{(q,i), (q',j)\}$$
 where  $q = q' \in \partial D$  and  $\psi_i = 2\alpha - \psi_i$ ,

where  $\alpha$  is the angle between e and the tangent vector to  $\partial D$  at q. Let  $p : U \to M$  be the unique set  $\omega \in M$  such that  $(q, i) \in \omega$ , which we denote [(q, i)]. We then give M the quotient topology.

Each set  $D(\psi_i)$  is naturally a smooth manifold with boundary. We suppose that on each  $D(\psi_i)$  a smooth structure is defined. It contains charts of the form  $(B, id_i)$  where  $id_i$  is the identity map on  $D(\psi_i)$  and B are balls which intersect at most a single side of the rhombus in  $D(\psi_i)$ . If  $q \notin \partial D$  then  $(B, id_i \circ p^{-1}(x))$  is a chart for M, where B is a small ball containing q, as described. If  $q \in \partial D$ , then let  $R_q : \mathbb{R}^2 \to \mathbb{R}^2$  be the reflection about the line parallel to  $\partial D$  at q. Let  $\sigma = \text{sign } n_q \cdot v(\psi_i)$  and  $S_q(x) = x - q$ , where  $S_q : \mathbb{R}^2 \to \mathbb{R}^2$ . A chart for M at q is then  $(B, \sum_{i:p^{-1}(B)\cap D(\psi_i)\neq\emptyset} R_q^{\sigma} \circ S_q \circ id_i \circ p^{-1}(x))$ . We introduce a smooth structure on M by taking the maximal smooth atlas containing all such charts.

As was shown in [25], there is a chart in a neighborhood of each corner of the rhombus. With these charts, the vector field  $v_{[(p,i)]} = v(\psi_i)$  on M is smooth and generates the billiard flow  $\Phi(x, t)$ . Any value of t is allowable which does not result in a trajectory running into a corner of the rhombus. We refer to the corner points of the rhombus as branch points.

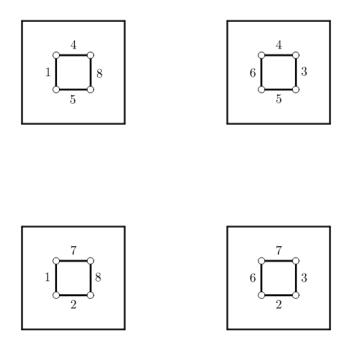


Figure 4.3: An illustration of M when the rhombus is a square. Edges with the same number are identified. The corners of the square are the branch points.

In a neighborhood of each corner point the flow is a local flow of parallel displacements, with a finite number of trajectories "entering" a branch point and a finite number of trajectories "exiting." We refer to any trajectory that enters or exits a branch point as a singular trajectory.

**Proposition 4.4.1.** On the manifold M there is a smooth function f such that fv is a vector field with the following properties:

- *fv* vanishes only at the branch points.
- The flow  $\tilde{\Phi}$  corresponding to fv is smooth.
- $\{\tilde{\Phi}(x,t)\}_{t=-\infty}^{\infty} = \{\Phi(x,t)\}_{t=-\infty}^{\infty}$ .
- The fixed points of the flow  $\tilde{\Phi}$  are the branch points.
- The flow in a neighborhood of each corner point is a saddle point.

To prove Proposition 4.4.1, one chooses a function f that vanishes in a neighborhood of each corner point and which is smooth with respect to the structure on M. The exact details can be found in [25].

**Corollary 4.4.1.** [25] Suppose the flow  $\Phi$  on M satisfies the following conditions:

- The number of singular points of the flow is finite.
- Each singular point is a saddle point with a finite number of entering and exiting separatrices.
- The non-wandering set of M coincides with M.
- $\Phi$  has no periodic trajectories.
- No separatrix of the flow  $\Phi$  goes from one singular point of the flow to another.

Then each positive or negative semitrajectory of the flow which is not a separatrix is dense in M.

**Proposition 4.4.2.** For almost all values of  $\psi$  the flow  $\tilde{\phi}$  satisfies the conditions of Corollary 4.4.1.

Again, the proof is entirely analogous to that in [25]. As a result of Proposition (4.4.1), for almost every x the trajectory determined by  $\Phi$  is dense in M.

A direct consequence of Proposition 4.4.2 is the following Corollary, whose proof is analogous to that presented in section 2 for Theorem 4.2.3.

**Corollary 4.4.2.** There is a dense set of points  $x \in \Omega(M, \Phi)$  for which the corresponding physical billiard hits vertices of the rhombus infinitely many times.

Hyperbolicity of these physical Wind-Tree models follows completely analogously to the considered above case of physical billiards in non-convex polygons.

**Theorem 4.4.3.** *The return map*  $\mathcal{F}$  *is hyperbolic.* 

#### 4.5 Statistical Properties of the Physical Wind-Tree Model

In this section we briefly discuss statistical properties of the physical wind-tree model. In particular, if the initial position of the particle is uniformly distributed with respect to the Liouville measure, then it is interesting to ask which functions f(t) are such that the following limit exists in distribution:

$$\lim_{t \to \infty} \frac{q_t - q_0}{f(t)}.\tag{4.2}$$

One may also ask a similar question regarding the return map  $\mathcal{F}$ . Denote  $(q_n, v_n) = \mathcal{F}^n(x)$ . For which functions f(n) does the following limit exist:

$$\lim_{n \to \infty} \frac{q_n - q_0}{f(n)}.$$

It is natural to make comparison with very well studied two dimensional periodic Lorentz gas. One places circles of fixed radius  $\alpha < 1/2$  at the points of some lattice, and considers the motion of a point particle reflecting from the scatterers (see figure 4.4). As was shown in [2] the limit indicated in 4.2 exists when  $f(t) = (t \ln t)^{1/2}$ , and gives a Gaussian distribution if a free path of the moving particle is bounded (so called finite horizon). If a free path is unbounded (infinite horizon) then convergence to the Gaussian distribution occurs under non-standard normalization  $(n \log n)^{1/2}$ .

The specific calculations used to arrive at these results for infinite horizon crucially involve analysis of trajectories that do not impact any of the circular scatterers for arbitrarily large amounts of time. Let L be any line that does not touch any of the scatterers and let n be any unit vector orthogonal to L. Set  $r^+ = \max\{\delta \ge 0 : L + tn$  does not touch any scatterer for  $0 < t < \delta\}$ , and let  $r^- = \max\{\delta \ge 0 : L - tn$  does not touch any scatter  $t < \delta\}$ . Then  $\bigcup_{r^- < t < r^+} L + tn$  is called a corridor. It is possible to show each sufficiently long free path lies almost entirely in some single corridor.

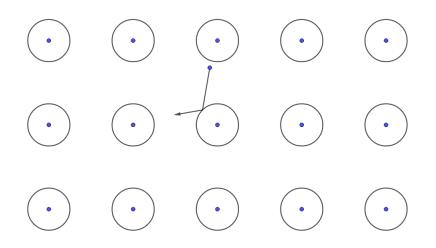


Figure 4.4: The periodic Lorentz gas with infinite horizon

For the periodic Lorentz gas there exist only one type of a corridor although this system may contain several of such similar corridors. For instance for the periodic lorentz gas depicted in Fig.4 there are three corridors. To the contrary for the physical Wind-Tree model, there are two distinctly different types of corridor. The first kind, with trajectories shown in figure 4.5, is bounded by two parallel straight lines tangent to rounded edges of the rhombus. Analysis of trajectories lying in such corridors seems to be similar to the analysis done for trajectories in the periodic Lorentz gas and present no special difficulties.

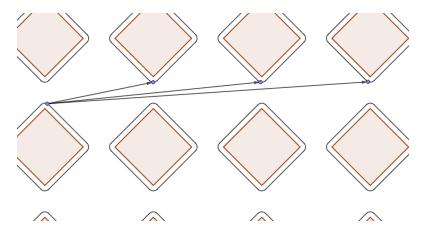


Figure 4.5: Trajectories in corridors of the first kind.

The second kind of corridor is shown in figure 4.6. Such corridors are bounded by parallel lines containing flat sides of the rhombuses.

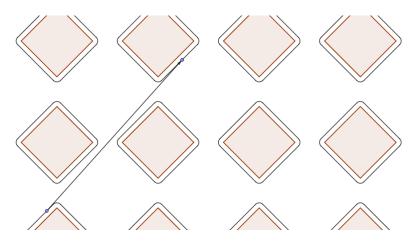


Figure 4.6: Trajectories in corridors of the second kind.

It is easy to built a physical Wind-Tree model with bounded free path, see e.g. the one depicted in figure 4.7.

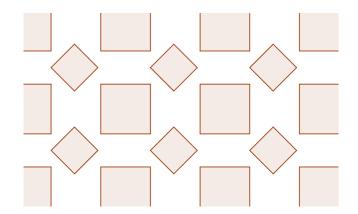


Figure 4.7: A physical Wind-Tree model without corridors.

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