
The Calkin-Wilf Tree and a Trace Condition

Master's Thesis



Julius-Maximilian's University of Würzburg
Faculty for Mathematics and Computer Science

by
Marc Philipp Technau
born in Freiburg im Breisgau

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Prof. Dr. Jörn Steuding

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Notations

$[a_0; a_1, \dots]$	continued fraction.
$\text{Aut}(\hat{\mathbb{C}})$	group of Möbius transformations on the Riemann sphere.
χ	see (A.3).
$e_m(z)$	$\exp(2\pi iz/m)$.
Γ	the Gamma-function.
γ	Euler-Mascheroni constant, $\gamma = 0.57721\dots$
$\mathcal{H}_{a,m}$	general modular hyperbola, see (2.14).
\mathcal{H}_m	modular hyperbola, see (2.1).
$K_m(r, s)$	Kloosterman sum, see (2.3).
$\mathbf{N}(n, m)$	see subsection 1.3.1.
$\mathcal{N}_m(\Omega)$	counting function for points contained in Ω and the modular hyperbola \mathcal{H}_m , see (2.2).
\mathbb{P}	the set of primes, $\mathbb{P} = \{2, 3, 5, 7, 11, \dots\}$.
$\varphi(m)$	number of $n, 1 \leq n \leq m$ relatively prime to m .
$\Phi(n)$	$\sum_{m=0}^{\infty} \mathbf{N}(n, m)$.
p_\bullet	(possibly finite) sequence p_k, p_{k+1}, \dots . The initial index k depends on the context.
$\Psi(N)$	$\sum_{3 \leq n \leq N} \Phi(n)$.
$\text{res}_{z_0} f$	residue of f at z_0 .
$\text{SL}_2\mathbb{Z}$	group of all 2×2 -matrices with integer coefficients and determinant 1.
$V_\alpha^\beta(f)$	total variation of the function f .
$\lfloor x \rfloor$	largest integer $\leq x$.
X^t	transpose of a matrix X .
ζ	the Riemann zeta-function.

Usual Conventions

We use the Landau symbol $O(\dots)$ and the Vinogradov symbol \ll . By writing $O_r(\dots)$ or \ll_r we mean to express that the implied constants are dependent on the parameter r (the range of this parameter will be obvious from the context in which it appears).

The symbol ε has a special meaning in the following sense: when writing $f(x) \ll_\varepsilon g_\varepsilon(x)$ or the $O_\varepsilon(\dots)$ -analogue these statements are claimed to hold for $\varepsilon > 0$ sufficiently small. However, they may not necessarily be valid if ε is taken too large (this is particularly relevant for the arguments in Section §3.2).

We briefly make use of the notation $O(m^{o(1)})$ in Section §2.3 which is understood to mean $O_\varepsilon(m^\varepsilon)$.

Preface

The examination regulations of Würzburg University require theses submitted in a language other than German to contain an abstract in German. We shall fulfill this requirement here. The reader may also find an english version below.

Zusammenfassung der Arbeit

Im Jahr 2000 führten Calkin und Wilf einen unendlichen binären Baum ein, welcher jede positive rationale Zahl genau einmal enthält. Dieser Baum kann iterativ generiert werden, indem man mit der Wurzel 1 beginnt und auf jeden Knoten zwei Möbiustransformationen anwendet, um dessen Kinder zu generieren. Durch Identifikation dieser Möbiustransformationen mit Matrizen erhält man einen unendlichen binären Matrix-wertigen Baum und eine natürliche Bijektion auf den Calkin-Wilf Baum.

In Kapitel 1 geben wir mehr Details zu der oben skizzierten Konstruktion und untersuchen die Verteilung von Zahlen im Calkin-Wilf Baum, welche zu Matrizen im Matrix-Baum gehören, die eine vorgegebene Spur haben. Die Zahlen $N(n, m)$, welche wir dabei einführen, konnten nicht in der On-Line Encyclopedia of Integer Sequences (OEIS) gefunden werden, was als Indiz dafür gelten kann, dass diese zuvor noch nicht untersucht wurden.

Dafür wurden jedoch die Funktionen

$$\Phi(n) := \sum_{m=0}^{\infty} N(n, m) \quad \text{und} \quad \Psi(N) := \sum_{n=3}^N \Phi(n)$$

zuvor von Kleban et al. (1999) eingeführt. Von Kleban et al. stammt die Vermutung

$$\Phi(n) \sim c \cdot n \log n \quad (c = 1).$$

Kallies et al. (2001) zeigten

$$\Psi(N) = \frac{1}{\zeta(2)} N^2 \log N + O(N^2 \log \log N).$$

Daraus ergibt sich, dass obige Vermutung modifiziert werden muss, um richtig zu sein. Tatsächlich müsste man $c = \frac{2}{\zeta(2)} = 1.21 \dots$ wählen. Peter (2001) konnte jedoch zeigen, dass auch diese modifizierte Vermutung falsch ist. Das bisher beste bekannte Ergebnis zu $\Psi(N)$ stammt von Boca (2007):¹

$$\Psi(N) = \underbrace{\frac{1}{\zeta(2)}}_{=0.607\dots} N^2 \log N + \underbrace{\frac{1}{\zeta(2)} \left(\gamma - \frac{3}{2} - \frac{\zeta'(2)}{\zeta(2)} \right)}_{=-0.214\dots} N^2 + O_{\varepsilon}(N^{\frac{7}{4}+\varepsilon}). \quad (0.1)$$

¹Im zugehörigen Artikel wird eine falsche Konstante vor dem N^2 -Term angegeben.

Kapitel 3 legt Bocas Resultat und dessen Beweis dar. Dabei korrigieren wir einige kleine Fehler im Originalartikel und weichen an manchen Stellen auch etwas von der Quelle ab. Insbesondere versuchen wir die geometrische Natur der zugrundeliegenden Ideen herauszukristallisieren und argumentieren mithilfe von Abbildungen, soweit dies hilfreich scheint.

Der Schlüssel zu Bocas Beweis ist die Reduktion des Problems $\Psi(N)$ zu berechnen auf ein Problem Punkte in modularen Hyperbeln in speziellen Regionen zu zählen, d.h. man versucht Punkte $(x, y) \in \mathbb{Z}^2 \cap \Omega$ mit $xy \equiv 1 \pmod{m}$ für feste $m \in \mathbb{N}$ und $\Omega \subseteq \mathbb{R}^2$ zu zählen. Dieses neue Problem lässt sich durch Anwenden bekannter Abschätzungen lösen.

In Kapitel 2 entwickeln wir diese Abschätzungen und widerlegen ein Resultat von Shparlinski (2012).

Damit wiederum gelingt in Kapitel 3 dann der Beweis der Formel

$$\Psi(N) = \sum_{m < N} \frac{\varphi(m)}{m^2} (N - m)^2 + O_\varepsilon(N^{\frac{7}{4} + \varepsilon}).$$

Obige Summe lässt sich anschließend, unter Benutzung einiger Resultate über die Riemannsche Zetafunktion, behandeln. Die dafür benötigten Hilfsmittel wurden im Anhang zusammengestellt.

Abstract

In 2000, Calkin and Wilf introduced an infinite binary tree which contains each positive rational number exactly once. This tree can be generated iteratively by starting with the root 1 and applying two Möbius transformations to each node to obtain its children. By identifying these Möbius transformations with corresponding matrices one obtains an infinite binary matrix-valued tree and a natural bijection onto the Calkin-Wilf tree.

In Chapter 1 we elaborate on the construction sketched above and subsequently investigate the distribution of numbers in the Calkin-Wilf tree which correspond to matrices in the matrix tree with fixed trace. The quantity $\mathbf{N}(n, m)$ introduced in the process could not be found within The On-Line Encyclopedia of Integer Sequences (OEIS), indicating that it was not studied previously.

However, the quantities

$$\Phi(n) := \sum_{m=0}^{\infty} \mathbf{N}(n, m) \quad \text{and} \quad \Psi(N) := \sum_{n=3}^N \Phi(n)$$

were introduced previously by Kleban and Özlük [1999] with mathematical physics in mind. They conjectured that

$$\Phi(n) \sim c \cdot n \log n \quad (c = 1).$$

Kallies et al. [2001] showed that

$$\Psi(N) = \frac{1}{\zeta(2)} N^2 \log N + O(N^2 \log \log N).$$

From this one finds that the above conjecture has to be modified, namely one has to take $c = \frac{2}{\zeta(2)} = 1.21\dots$; however, as shown by Peter [2001], even this modified conjecture is wrong. The so far best result concerning $\Psi(N)$ is due to Boca [2007],²

$$\Psi(N) = \underbrace{\frac{1}{\zeta(2)}}_{=0.607\dots} N^2 \log N + \underbrace{\frac{1}{\zeta(2)} \left(\gamma - \frac{3}{2} - \frac{\zeta'(2)}{\zeta(2)} \right)}_{=-0.214\dots} N^2 + O_\varepsilon(N^{\frac{7}{4} + \varepsilon}). \quad (0.2)$$

²In the paper an erroneous value for the term in front of N^2 is given.

Chapter 3 is devoted to giving an exposition of Bocas result. We correct some minor errors in the process and deviate from the original exposition at several stages. In particular, we try to stress the geometric nature of some of the main ideas and choose to appeal to figures where it seems helpful.

The key ingredient to Bocas proof is reducing the problem of calculating $\Psi(N)$ to a problem of counting points on modular hyperbolas in certain shapes, that is counting points $(x, y) \in \mathbb{Z}^2 \cap \Omega$ such that $xy \equiv 1 \pmod{m}$ for given $m \in \mathbb{N}$ and $\Omega \subseteq \mathbb{R}^2$. This new problem is subsequently solved by applying known estimates.

In Chapter 2 we develop these estimates and disprove a result found in [Shparlinski, 2012].

Back in Chapter 3 we obtain the formula

$$\Psi(N) = \sum_{m < N} \frac{\varphi(m)}{m^2} (N - m)^2 + O_\varepsilon(N^{\frac{7}{4} + \varepsilon})$$

from the aforementioned reduction and the estimates from Chapter 2. The above sum is dealt with by appealing to some facts about the Riemann zeta function. The necessary tools are presented in the appendix.

Outlook

On the Error Term in the Formula for $\Psi(N)$

We shall make some remarks on the $\frac{7}{4}$ -boundary in the error term in (0.2). Reduced to its very core Bocas argument gives a formula of the type

$$\Psi(N) = \sum_{m < N} \#\text{hyperbola points mod } m \text{ in the region } \Omega_{N,m},$$

where $\Omega_{N,m}$ is a region depending on N and m . The number of hyperbola points (mod m) in a rectangular region can be controlled up to an error of $O_\varepsilon(m^{\frac{1}{2} + \varepsilon})$. In order to obtain an estimate for the number of hyperbola points (mod m) in $\Omega_{N,m}$ the region is approximated by $\lfloor N^{\frac{1}{4}} \rfloor$ rectangles (the exponent $\frac{1}{4}$ is optimal for this particular problem). Therefore, one already has an error of $O_\varepsilon(N^{\frac{1}{4}} m^{\frac{1}{2} + \varepsilon})$. Summing over $m < N$ this gives an error of

$$O_\varepsilon(N(N^{\frac{1}{4}} N^{\frac{1}{2} + \varepsilon})) = O_\varepsilon(N^{\frac{7}{4} + \varepsilon}).$$

Since no improvement on the error $O_\varepsilon(m^{\frac{1}{2} + \varepsilon})$ for rectangular regions is to be expected one might hope to obtain better results by proving estimates custom-tailored for the regions $\Omega_{N,m}$ (note, that these do not look all too complicated, see Chapter 3 for details). Preliminary approaches, by trying to adapt the method used to prove the estimate for rectangular regions, proved to be fruitless. In fact, one encounters exactly the problems that are touched upon in Section §2.3, but the easy shape of the regions $\Omega_{N,m}$ may still save the underlying arguments.

More on the Quantity $\mathbf{N}(n, m)$

The inquiry conducted on the quantity $\mathbf{N}(n, m)$ in Chapter 1 still only scratches the surface of what might be possible. From what we show in this thesis one already obtains $\Phi(n) = 2\mathbf{N}(n, 0)$. Since estimating $\Phi(n)$ was already of interest prior to this thesis this might motivate further investigation on $\mathbf{N}(n, m)$.

In particular, we prove in Chapter 3 that $\mathbf{N}(n, m)$ is monotonically decreasing as m increases (for n fixed). It would be interesting to know for which m we have a jump, namely $\mathbf{N}(n, m) > \mathbf{N}(n, m + 1)$. Now, given a jump point (n, m) , can one find non-trivial estimates for the time k

up to the next jump,

$$\mathbf{N}(n, m) > \mathbf{N}(n, m + 1) = \dots = \mathbf{N}(n, m + k) > \mathbf{N}(n, m + k + 1) \geq 1 ?$$

Words of Appreciation

At this point some words of appreciation might be appropriate. The author would like to thank Prof. Dr. Steuding, first and foremost, for his constant encouragement in the times when unexpected obstacles shattered new ideas, but also for his advice, thorough reading of this thesis and giving the author the opportunity of speaking on this subject at the AaA7-workshop.

Also, the author would like to thank his cousin Niclas with whom he had the great pleasure of spending his first 10 years growing up together and eventually also studying mathematics together. His support, friendship and all ensuing mathematical discussions with him have proven to be invaluable to the author.

Chapter 1

The Calkin-Wilf Tree and a Trace Condition

1.1 The Calkin-Wilf Tree

We start this inquiry by recalling some well-known facts. Given a matrix $X = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2\mathbb{Z}$ we associate with it the Möbius transformation

$$m_X : z \mapsto \frac{az + b}{cz + d}.$$

This induces an epimorphism of groups

$$\mathrm{SL}_2\mathbb{Z} \longrightarrow \Gamma := \left\{ z \mapsto \frac{az + b}{cz + d} \mid a, b, c, d \in \mathbb{Z}, ad - bc = 1 \right\} \subseteq \mathrm{Aut}(\hat{\mathbb{C}})$$

with kernel $\{\pm 1\}$, whence $\mathrm{PSL}_2\mathbb{Z} := \mathrm{SL}_2\mathbb{Z}/\{\pm 1\} \cong \Gamma$.

Since Γ acts naturally on $\hat{\mathbb{C}}$ by evaluation, so does $\mathrm{SL}_2\mathbb{Z}$ by means of the above homomorphism. We are particularly interested in the evaluation at 1, so it will be useful to assign a name to the map

$$\tau : \mathrm{SL}_2\mathbb{Z} \longrightarrow \hat{\mathbb{C}}, \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} = X \mapsto m_X(1) = \frac{a + b}{c + d}.$$

More generally, by replacing the evaluation at 1 by the evaluation at some other point $\alpha \in \mathbb{R}_+$, we are inclined to consider the maps

$$\tau_\alpha : \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto \frac{a\alpha + b}{c\alpha + d}.$$

We will make some remarks on their interplay in due time.

Now, consider the matrices

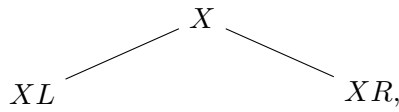
$$L := \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad R := L^t = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}.$$

It is commonly known that the monoid

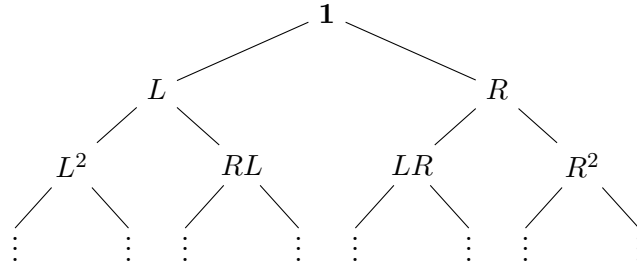
$$\mathcal{M} := \{A_1 \cdots A_r \mid r \in \mathbb{N}_0, A_1, \dots, A_r \in \{L, R\}\}$$

generated by L and R is free over $\{L, R\}$, see e.g. Calkin and Wilf [2000] or Nathanson [2014] for stronger results (the empty product $A_1 \cdots A_r$ for $r = 0$ is understood to mean $\mathbf{1}$). In the remainder of the chapter when writing $A_1, A_2 \dots$ these objects are always understood to be either L or R . Thus, by writing $X = A_1 \cdots A_r$ we contend that the right hand side is the (unique) expression of X as product of L s and R s.

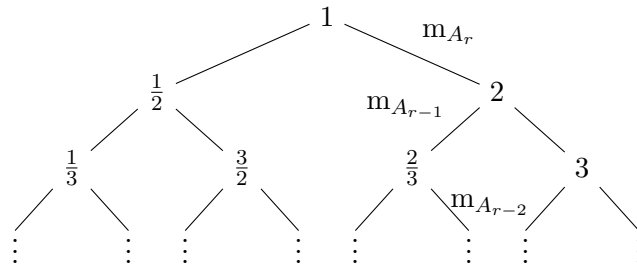
The fact that \mathcal{M} is free over $\{L, R\}$ is reflected in the observation that each element $A_1 \cdots A_r$ appears exactly once in the binary tree \mathcal{T} with root $\mathbf{1}$ and generation rule



that is, the tree



Given an element $X = A_1 \cdots A_r \in \mathcal{M}$ we have an associated element $\tau(X) \in \hat{\mathbb{C}}$. In fact, one immediately verifies $\tau(X) \in \mathbb{Q}_+$. So, by applying the map τ to each node of the above tree \mathcal{T} we obtain yet another binary tree \mathcal{T}_1 :



This so called Calkin-Wilf tree was introduced by Calkin and Wilf [2000]. They showed that each number $x \in \mathbb{Q}_+$ appears once and only once within this tree, i.e. the map

$$\tau|_{\mathcal{M}} : \mathcal{M} \longrightarrow \mathbb{Q}_+ \tag{1.1}$$

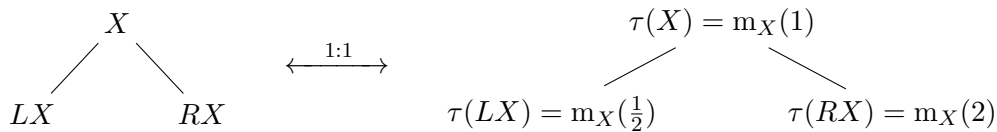
is a bijection.¹

Now, fix $\beta \in \mathbb{Q}_+$ and let $B := \tau^{-1}(\beta)$. Because of

$$\tau_\beta(X) = m_X(\beta) = m_X(\tau(B)) = m_X(m_B(1)) = m_{XB}(1) = \tau(XB),$$

we find that the tree \mathcal{T}_β obtained by applying τ_β to the tree \mathcal{T} is contained in \mathcal{T}_1 as a subtree, namely the image of the subtree with node B of \mathcal{T} under $\tau = \tau_1$. This, in some sense, justifies the special place we have attributed to the map τ_1 amongst all the other maps τ_β for $\beta \in \mathbb{Q}_+$. Theory for understanding the case $\beta \in \mathbb{R}_+ \setminus \mathbb{Q}$ are developed Sander et al. [2011].

The fact that (1.1) is a bijective map immediately gives rise to a certain field of problems: by virtue of the association



¹The resulting enumeration of \mathbb{Q}_+ when reading the tree row by row was actually investigated previously by Stern [1858]; see also the remarks in Calkin and Wilf [2000].

one can assign a number $x \in \mathbb{Q}_+$ a property of the matrix $\tau^{-1}(x) \in \mathcal{M}$. Now, given a certain property, what are the numbers $x \in \mathbb{Q}_+$ such that $\tau^{-1}(x)$ admits this property? Questions concerning the distribution and statistical properties of such numbers may also be of interest.

Inquiry on questions of this type is by no means new. For instance, Alkauskas and Steuding [2007] investigate properties of numbers $\tau(X)$, where X is chosen from one fixed row of the tree. The corresponding matrix-property is $h(X) = \text{const}$, where

$$h : \mathcal{M} \longrightarrow \mathbb{N}_0, \quad A_1 \cdots A_r \longmapsto r \quad (1.2)$$

gives the height of the element $A_1 \cdots A_r$ in the tree. In particular Alkauskas and Steuding [2007] prove

$$\sum_{X \in h^{-1}(r)} \tau(X) = 3 \cdot 2^{r-1} - \frac{1}{2},$$

which immediately yields an expression for the average value of τ on the set $h^{-1}(r)$, since there are precisely 2^r elements in $h^{-1}(r)$; a stronger result of this type is due to Reznick [2008]. See also Sander et al. [2011, Theorem 3] for a generalization of this.

Our main focus lies on the case where the property in question boils down to some kind of restriction on the trace of the matrix $\tau^{-1}(x)$. Elaboration on this thought will follow shortly.

1.2 Relation to Continued Fractions

In order to further investigate the relation between \mathcal{M} and \mathbb{Q}_+ we must first better understand the nature of the products $A_1 \cdots A_r$. The results presented in the present section may be found in Kallies et al. [2001] and in Boca [2007]. We follow closely the exposition in Einsiedler and Ward [2010, Ch. 3] and Boca [2007].

1.2.1. Some Facts about Continued Fractions

Every number $x \in \mathbb{R}_+$ has a continued fraction expansion

$$x = a_0 + \frac{1}{a_1 + \frac{1}{a_2 + \cdots}} =: [a_0; a_1, a_2, \dots],$$

where $a_1, a_2, \dots \in \mathbb{N}$ and $a_0 = [x]$ is the integer part of x (this expansion can be generated by the Gauß map, see Einsiedler and Ward [2010, Ch. 3] for details). If x is rational then a_\bullet is finite, i.e. $a_\bullet = (a_1, \dots, a_n)$. Apart from the ambiguity

$$[a_0; a_1, \dots, a_{n-1}, a_n, 1] = [a_0; a_1, \dots, a_{n-1}, a_n + 1]$$

this representation is unique.

When one is given $a_1, \dots, a_n \in \mathbb{N}$ and $a_0 \in \mathbb{N}_0$ these numbers determine a rational number

$$[a_0; a_1, \dots, a_n] = \frac{p_n}{q_n},$$

where the fraction $\frac{p_n}{q_n}$ is assumed to be in lowest terms with $p_n \in \mathbb{N}_0$ and $q_n \in \mathbb{N}$.

The numbers p_n, q_n appear as coefficients in the matrix

$$\begin{pmatrix} p_n & p_{n-1} \\ q_n & q_{n-1} \end{pmatrix} = M(a_0)M(a_1) \cdots M(a_n), \quad (1.3)$$

where

$$M(a) := \begin{pmatrix} a & 1 \\ 1 & 0 \end{pmatrix}$$

and $p_{-1} := 1, q_{-1} := 0$. Note that $p_0 = a_0$ and $q_0 = 1$. From this we may easily deduce the recursive formulas

$$\begin{cases} p_{n+1} = a_{n+1}p_n + p_{n-1}, \\ q_{n+1} = a_{n+1}q_n + q_{n-1}. \end{cases} \quad (1.4)$$

Applying the determinant to (1.3) we obtain

$$p_n q_{n-1} - p_{n-1} q_n = (-1)^{n+1}.$$

By means of (1.4) the numbers q_{n-1} and q_n are easily seen to be coprime. For their quotient we have the identity

$$\frac{q_{n-1}}{q_n} = \frac{q_{n-1}}{a_n q_{n-1} + q_{n-2}} = \frac{1}{a_n + \frac{q_{n-2}}{q_{n-1}}} = \dots = \frac{1}{a_n + \frac{1}{a_{n-1} + \frac{1}{\dots + a_1}}} = [0; a_n, \dots, a_1].$$

1.2.2. Relation to Products of L s and R s

For $l, r \in \mathbb{Z}$ one easily verifies the identities

$$L^l = \begin{pmatrix} 1 & 0 \\ l & 1 \end{pmatrix} \quad \text{and} \quad R^r = \begin{pmatrix} 1 & r \\ 0 & 1 \end{pmatrix} \quad (1.5)$$

and we obtain

$$R^r L^l = M(r)M(l).$$

For numbers $a_1, \dots, a_{2m} \in \mathbb{N}$ and $a_0 := 0$ and p_\bullet, q_\bullet defined as previously, combining this with (1.3) and writing

$$J := M(0) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (1.6)$$

this yields

$$R^{a_1} L^{a_2} \dots R^{a_{2m-1}} L^{a_{2m}} = M(a_1) \dots M(a_{2m}) = J \begin{pmatrix} p_{2m} & p_{2m-1} \\ q_{2m} & q_{2m-1} \end{pmatrix} = \begin{pmatrix} q_{2m} & q_{2m-1} \\ p_{2m} & p_{2m-1} \end{pmatrix}. \quad (1.7)$$

Since we have the identity

$$R^r = J L^r J = J^{-1} L^r J.$$

equation (1.7) transforms into

$$L^{a_1} R^{a_2} \dots L^{a_{2m-1}} R^{a_{2m}} = J \begin{pmatrix} q_{2m} & q_{2m-1} \\ p_{2m} & p_{2m-1} \end{pmatrix} J = \begin{pmatrix} p_{2m-1} & p_{2m} \\ q_{2m-1} & q_{2m} \end{pmatrix}.$$

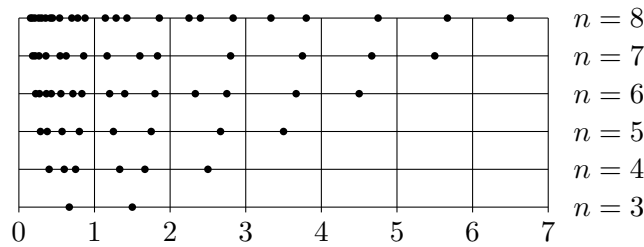
Again, using (1.5), equation (1.7) gives more identities, namely

$$\begin{aligned} R^{a_1} L^{a_2} \dots R^{a_{2m-1}} L^{a_{2m}} R^{a_{2m+1}} &= \begin{pmatrix} q_{2m} & q_{2m-1} \\ p_{2m} & p_{2m-1} \end{pmatrix} \begin{pmatrix} 1 & a_{2m+1} \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} q_{2m} & q_{2m+1} \\ p_{2m} & p_{2m+1} \end{pmatrix}, \\ L^{a_1} R^{a_2} \dots L^{a_{2m-1}} R^{a_{2m}} L^{a_{2m+1}} &= J \begin{pmatrix} q_{2m} & q_{2m+1} \\ p_{2m} & p_{2m+1} \end{pmatrix} J = \begin{pmatrix} p_{2m+1} & p_{2m} \\ q_{2m+1} & q_{2m} \end{pmatrix}. \end{aligned}$$

The above identities are of little interest to us for the remainder of the inquiry in this chapter, as we now shift our focus back onto trace conditions. However, these identities will be of great interest when we take a more in depth look into the paper [Boca, 2007] in Chapter 3. We merely chose to develop this machinery at the present point, because it seemed to fit the flair of the current investigation.

1.3 Locating Elements with fixed associated Trace

In this section we will study the frequency of integer parts of $\tau(X)$ for $X \in \mathcal{M}$ subject to the restriction $\text{tr } X = n$, where $n \in \mathbb{N}$ is fixed.² As a motivation we plot the points $\{\tau(X) \mid X \in \mathcal{M}, \text{tr } X = n\}$ for $n = 3, \dots, 8$ and arrive at the following figure:



Obviously, for $m \in \mathbb{N}_0$ the numbers $\tau(X)$ seem to cluster within the intervals $[m, m + 1)$ with their total amount decreasing as m increases. We will give a proof of this fact shortly amongst other properties which one may conjecture when looking at the above figure.

1.3.1. First Observations

We shall denote the numbers of our interest by

$$N(n, 0), N(n, 1), N(n, 2), \dots,$$

where $N(n, m)$ is defined as

$$N(n, m) := \#\{X \in \mathcal{M} \mid \text{tr } X = n, \tau(X) \in [m, m + 1)\}.$$

We first look into the case $n = 2$. Observe that each of the matrices L^k and R^k for $k \in \mathbb{N}_0$ has trace 2; one easily verifies the identities $\tau(L^k) = \frac{1}{k+1}$ and $\tau(R^k) = k + 1$. We contend that the aforementioned matrices are the only matrices in \mathcal{M} with trace 2. To verify this, consider the identities

$$\text{tr} \left[\begin{pmatrix} a & b \\ c & d \end{pmatrix} L \right] = \text{tr} \begin{pmatrix} a & b \\ c & d \end{pmatrix} + b \quad \text{and} \quad \text{tr} \left[\begin{pmatrix} a & b \\ c & d \end{pmatrix} R \right] = \text{tr} \begin{pmatrix} a & b \\ c & d \end{pmatrix} + c. \quad (1.8)$$

Combining these with $\text{tr}(LR) = 3$ we conclude that $X \in \mathcal{M}$ has trace ≥ 3 whenever X is of the form

$$X = Y_1 L R Y_2 \quad \text{or} \quad X = Y_1 R L Y_2 \quad (1.9)$$

for some $Y_1, Y_2 \in \mathcal{M}$.

Indeed, we can easily conclude more: say (1.9) holds. We will only deal with the case $X = Y_1 L R Y_2$ for simplicity's sake; the other case can be treated in the same fashion. Since the trace

²One may also ask what happens when requiring X to have prescribed eigenvalues. Since X has the characteristic polynomial $Y^2 - (\text{tr } X)Y + 1 \in \mathbb{R}[Y]$ prescribing $\text{tr } X = n$ amounts to prescribing the eigenvalues to be $\frac{n}{2} \pm \frac{1}{2}\sqrt{n^2 - 4}$ and vice versa.

is invariant under cyclic permutations we get

$$\operatorname{tr} X = \operatorname{tr} (LRY_2Y_1).$$

Decomposing $Y_2Y_1 = A_1 \cdots A_{r-2}$ and invoking (1.8) we infer

$$\operatorname{tr} X \geq r + 1, \tag{1.10}$$

where obviously the quantity r is the length of the decomposition of X into a product of L s and R s. In particular, for fixed $n \geq 3$ there can only exist finitely many $X \in \mathcal{M}$ such that $\operatorname{tr} X = n$, since from a certain height upward in the tree there are only matrices having trace $> n$ or matrices of the form L^k, R^k , whose trace clearly is $2 \neq n$, as observed previously.

Gathering what we have proved so far, we may state

Theorem 1.1. Let $n \in \mathbb{N}$ and $m \in \mathbb{N}_0$. Then the following statements hold:

- (a) $\mathbf{N}(2, 0) = \infty$,
- (b) $\mathbf{N}(2, 1 + m) = 1$,
- (c) $\mathbf{N}(2 + n, m) < \infty$.

1.3.2. The Case $m \geq 3$

In view of Theorem 1.1 we direct our attention to the only remaining interesting case, i.e. $\mathbf{N}(n, m)$ where $n \geq 3$. At the beginning of the chapter we have mentioned that the map

$$\operatorname{SL}_2\mathbb{Z} \longrightarrow \Gamma, \quad X \longmapsto m_X$$

is a homomorphism. We use this property to obtain

$$\tau(A_1 \cdots A_r) = m_{A_1 \cdots A_r}(1) = (m_{A_1} \circ \cdots \circ m_{A_r})(1),$$

whence understanding what τ does to $X \in \mathcal{M}$ reduces to understanding the mapping properties of m_L and m_R . To this end turning to continued fractions seems expedient; indeed, as used by Sander et al. [2011] and mentioned by Alkauskas [2008], the maps m_L and m_R adhere to the following property:

Lemma 1.2. Let $x \in \mathbb{R}_+$ be given by its continued fraction expansion $x = [a_0; a_1, \dots]$. Then one has

$$m_R(x) = [a_0 + 1; a_1, \dots], \quad \text{and} \quad m_L(x) = \begin{cases} [0; a_1 + 1, a_2, \dots], & x \leq 1, \\ [0; 1, a_0, a_1, \dots], & x > 1. \end{cases}$$

PROOF: The statement for m_R is evident. Now suppose $x < 1$ and let $y = [a_2; a_3, \dots]$. Then we have $x = [0; a_1, y]$ and a direct calculation yields

$$m_L(x) = \frac{x}{x+1} = \frac{1}{a_1 + 1 + \frac{1}{y}} = [0; a_1 + 1, a_2, \dots].$$

The case $x > 1$ is proved in the same way and the case $x = 1$ is easily verified. ■

In the case $(r, a_1) \neq (1, 1)$ one has

$$[[a_0; a_1, \dots, a_r]] = a_0.$$

We proceed by putting Lemma 1.2 to good use in proving the following

Theorem 1.3. Let $n \geq 3$. Then the following statements hold:

- (a) $\mathbf{N}(n, n-1) = \mathbf{N}(n, n) = \dots = 0$,
- (b) $\mathbf{N}(n, n-2) = 1$,
- (c) $\mathbf{N}(n, 0) = \sum_{m=1}^{n-2} \mathbf{N}(n, m)$,
- (d) $\mathbf{N}(n, 0) \geq \mathbf{N}(n, 1) \geq \dots \geq \mathbf{N}(n, n-1)$.

PROOF: It will be convenient to write

$$\mathcal{M}_n := \{X \in \mathcal{M} \mid \text{tr } X = n\}.$$

- (a) Let $X \in \mathcal{M}$. By means of the decomposition $X = A_1 \cdots A_r$, the identity

$$\tau(X) = m_{A_1} \circ \cdots \circ m_{A_r}(1)$$

and by appealing to Lemma 1.2 we conclude that $\tau(X)$ is maximal amongst all $\tau(h^{-1}(r)) \subseteq \mathbb{Q}_+$ if and only if $A_1 = \dots = A_r = R$, i.e. $X = R^r$, h being the function from (1.2).

If we additionally require $\text{tr } X \neq 2$ and thus seek the maximal value M_r of $\tau(h^{-1}(r) \setminus \mathcal{M}_2)$ then we arrive, again by Lemma 1.2, at the conclusion that this maximum is only attained for

$$X = R^{r-1}L = \begin{pmatrix} r & r-1 \\ 1 & 1 \end{pmatrix}. \quad (1.11)$$

This in turn yields $M_r = r - \frac{1}{2}$. Note that $\text{tr } X = r + 1$.

If we now seek to maximize $\tau(X)$ for $X \in \mathcal{M}_n$ we need only observe that by (1.10) one has $h(X) \leq n - 1$ and hence

$$\mathcal{M}_n \subseteq \bigcup_{r=0}^{n-1} h^{-1}(r) \setminus \mathcal{M}_2.$$

The maximal value of $\tau(X)$ for X chosen from the set on the right hand side was previously seen to be $n - \frac{3}{2} \in [n-2, n-1)$, being attained by X as in (1.11) for $r = n-1$. In particular this X has trace n and we conclude $\mathbf{N}(n, m) = 0$ for every $m \geq n-1$, as desired.

(b) We have just seen that the matrix $R^{n-2}L$ contributes to $\mathbf{N}(n, n-2)$, so evidently we have $\mathbf{N}(n, n-2) \geq 1$. Now, we need only verify that no other matrix from \mathcal{M} makes a contribution to $\mathbf{N}(n, n-2)$. Equivalently, we mean to show

$$M'_n := \max \tau(\mathcal{M}_n \setminus \{R^{n-2}L\}) < n - 2. \quad (1.12)$$

Using similar arguments to those from the proof of (a), we conclude that the matrices $R^{n-3}LR$ and $R^{n-3}LL$ satisfy

$$M'_n \leq \min\{\tau(R^{n-3}LR), \tau(R^{n-3}LL)\}. \quad (1.13)$$

By appealing to the identities

$$R^{n-3}LR = \begin{pmatrix} n-2 & 2n-5 \\ 1 & 2 \end{pmatrix} \quad \text{and} \quad R^{n-3}LL = \begin{pmatrix} 2n-5 & n-3 \\ 2 & 1 \end{pmatrix}$$

we see that $R^{n-3}LL$ fails to meet the trace condition for $n \neq 4$. In any case we have

$$\tau(R^{n-3}LL) = n - \frac{8}{3} < \tau(R^{n-3}LR) = n - \frac{7}{3} < n - 2,$$

Chapter 2

Modular Hyperbolas

2.1 Preparatory Facts

The present chapter has the main purpose of providing necessary machinery for the discussion in Chapter 3. We start by collecting several facts from Shparlinski [2012].

Given $m \in \mathbb{N}$ we are interested in the location of points on the modular hyperbola

$$\mathcal{H}_m := \{(x, y) \in \mathbb{Z}^2 \mid xy \equiv 1 \pmod{m}\}. \quad (2.1)$$

In particular, we seek to find good estimates for the number of such points lying in a given region $\Omega \subseteq \mathbb{R}^2$, that is,

$$\mathcal{N}_m(\Omega) := \#\{(x, y) \in \mathcal{H}_m \cap \Omega\}. \quad (2.2)$$

As it turns out, Kloosterman sums are the canonical tool for studying such a problem. Abbreviating

$$e_m(z) := \exp(2\pi iz/m),$$

the (complete) Kloosterman sum $K_m(r, s)$ is given by

$$K_m(r, s) := \sum_{\substack{(x, y) \in \mathcal{H}_m \\ 1 \leq x, y \leq m}} e_m(rx + sy). \quad (2.3)$$

When requiring $m = p$ to be prime one has the bound

$$|K_p(r, s)| \leq 2\sqrt{p}$$

due to Weil [1948]. For not necessarily prime m one has the bound

$$|K_m(r, s)| \leq \tau(m)(m \gcd(r, s, m))^{\frac{1}{2}},$$

(see Iwaniec and Kowalski [2004, Corollary 11.12]), where $\tau(m)$ denotes the number of (positive) divisors of m . Using standard estimates on $\tau(m)$ one obtains

$$|K_m(r, s)| \ll_{\varepsilon} (m \gcd(r, s, m))^{\frac{1}{2} + \varepsilon}. \quad (2.4)$$

As a consequence of the formula for sums over geometric progressions we obtain

$$\sum_{r=W+1}^Z e_m(rx) = e_m(x(W+1)) \cdot \frac{1 - e_m(xZ)}{1 - e_m(x)} \quad (2.5)$$

for any $W, Z, x \in \mathbb{Z}$ such that $e_m(x) \neq 1$ (i.e. $m \nmid x$). In the case $(W, Z) = (0, m)$ this reduces

to a well-known orthogonality property of characters, namely

$$\frac{1}{m} \sum_{r=1}^m e_m(rx) = \begin{cases} 1, & \text{if } x \equiv 0 \pmod{m}, \\ 0, & \text{if } x \not\equiv 0 \pmod{m}. \end{cases} \quad (2.6)$$

For the modulus of (2.5) we find that

$$\left| \sum_{r=W+1}^{W+Z} e_m(rx) \right| \leq \frac{1}{|1 - e_m(x)|} = \frac{1}{|\exp(\pi ix/m) - \exp(-\pi ix/m)|} = \frac{1}{2|\sin(\pi x/m)|}.$$

Assuming $|x| \leq \frac{m}{2}$, we arrive at the estimate

$$\left| \sum_{r=W+1}^{W+Z} e_m(rx) \right| \leq \min \left\{ Z, \frac{m}{4|x|} \right\} \leq \min \left\{ Z, \frac{m}{2(|x|+1)} \right\}. \quad (2.7)$$

2.2 Distribution of Hyperbola Points

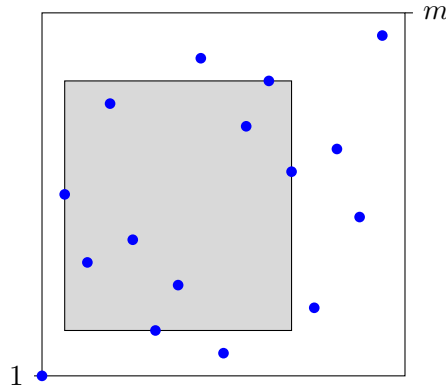
2.2.1. Distribution in Rectangles

We shift our attention back to estimating $\mathcal{N}_m(\Omega)$. In particular, we consider the case where Ω is a rectangle. The following theorem and its proof are taken from Shparlinski [2012].

Theorem 2.1. Let $\mathcal{X} = \{U+1, \dots, U+X\}$ and $\mathcal{Y} = \{V+1, \dots, V+Y\}$, where $m > X, Y \geq 1$ and $U \geq 0$ are arbitrary integers. Then we have

$$\mathcal{N}_m(\mathcal{X} \times \mathcal{Y}) = \frac{\varphi(m)}{m^2} XY + O_\varepsilon(m^{\frac{1}{2}+\varepsilon}). \quad (2.8)$$

Note, that XY is the area of the rectangle $(U, U+X] \times (V, V+Y]$.



PROOF: Using (2.6) twice, rearranging terms and using the definition (2.3) of Kloosterman sums we find that

$$\begin{aligned} \mathcal{N}_m(\mathcal{X} \times \mathcal{Y}) &= \sum_{\substack{(x,y) \in \mathcal{H}_m \\ x \in \mathcal{X}, y \in \mathcal{Y}}} 1 = \frac{1}{m^2} \sum_{\substack{(x,y) \in \mathcal{H}_m \\ 1 \leq x, y \leq m}} \sum_{w \in \mathcal{X}} \sum_{z \in \mathcal{Y}} \sum_{r,s=1}^m e_m(r(x-w) + s(y-z)) \\ &= \frac{1}{m^2} \sum_{r,s=1}^m K_m(r, s) \sum_{w \in \mathcal{X}} e_m(-rw) \sum_{z \in \mathcal{Y}} e_m(-sz). \end{aligned}$$

The terms corresponding to $r = s = m$ add up to

$$\frac{1}{m^2} K_m(m, m) \sum_{w \in \mathcal{X}} \sum_{z \in \mathcal{Y}} 1 = \frac{1}{m^2} XY \sum_{\substack{(x,y) \in \mathcal{H}_m \\ 1 \leq x,y \leq m}} 1 = \frac{\varphi(m)}{m^2} XY,$$

which is precisely the main term in (2.8).

The sum over the remaining terms, denoted by \mathcal{E}_m , can be treated using (2.4):

$$|\mathcal{E}_m| \ll_{\varepsilon} m^{-\frac{3}{2}+\varepsilon} \sum_{r,s=1}^{m-1} \gcd(r, s, m)^{\frac{1}{2}+\varepsilon} \left| \sum_{w=U+1}^{U+X} e_m(-rw) \sum_{z=V+1}^{V+Y} e_m(-sz) \right|. \quad (2.9)$$

Since all terms in r and s yield the same value if r and s are replaced by any other representative from the residue classes $r + m\mathbb{Z}$ and $s + m\mathbb{Z}$ respectively, we might as well just replace the sum

$$\sum_{r,s=1}^{m-1} \quad \text{with the sum} \quad \sum_{-\frac{m}{2} < r,s \leq \frac{m}{2}},$$

which in turn makes (2.7) applicable. Applying (2.7) and grouping the summands with the same value $\gcd(r, s, m) = d$ together yields¹

$$\begin{aligned} |\mathcal{E}_m| &\ll_{\varepsilon} m^{\frac{1}{2}+\varepsilon} \sum_{\substack{d|m \\ d \neq m}} d^{\frac{1}{2}+\varepsilon} \sum_{\substack{-\frac{m}{2} < r,s \leq \frac{m}{2} \\ \gcd(r,s,m)=d}} \frac{1}{4(|r|+1)(|s|+1)} \\ &\ll_{\varepsilon} m^{\frac{1}{2}+2\varepsilon} \sum_{\substack{d|m \\ d \neq m}} d^{\frac{1}{2}} \left(\left(\sum_{-\frac{m}{2d} < t \leq \frac{m}{2d}} \frac{1}{d|t|+1} \right)^2 - 1 \right) \end{aligned} \quad (2.10)$$

The innermost sum is easily estimated using Riemann sums:

$$\sum_{-\frac{m}{2d} < t \leq \frac{m}{2d}} \frac{1}{d|t|+1} < 1 + \sum_{1 \leq t \leq \frac{m}{2d}} \frac{2}{dt+1} \leq 1 + \int_0^{\frac{m}{2d}} \frac{2}{dt+1} dt = 1 + \frac{2 \log(\frac{m}{2} + 1)}{d},$$

whence showing

$$|\mathcal{E}_m| \ll_{\varepsilon} m^{\frac{1}{2}+2\varepsilon} \sum_{\substack{d|m \\ d \neq m}} d^{-\frac{1}{2}} \ll_{\varepsilon} m^{\frac{1}{2}+3\varepsilon}.$$

Since $\varepsilon > 0$ can be chosen arbitrarily we can also write

$$|\mathcal{E}_m| \ll_{\varepsilon} m^{\frac{1}{2}+\varepsilon}. \quad \blacksquare$$

Theorem 2.1 extends readily to rectangular regions whose side's lengths exceed m . Indeed, if given $\mathcal{X} = \{U+1, \dots, U+X\}$ and $\mathcal{Y} = \{V+1, \dots, V+Y\}$ where X, Y need only obey $X, Y \geq 1$ we can partition \mathcal{X} into $1 + \lfloor \frac{X}{m} \rfloor$ groups

$$\underbrace{U+1, \dots, U+m-1}, \underbrace{U+m, \dots, U+2m-1}, \dots$$

By doing the same with \mathcal{Y} we obtain a decomposition of the rectangle $(U, U+X] \times (V, V+Y]$ into $(1 + \lfloor \frac{X}{m} \rfloor)(1 + \lfloor \frac{Y}{m} \rfloor)$ rectangles of a suitable size for Theorem 2.1 to be applicable. The main

¹Notice, that Shparlinski [2012] is missing the -1 term after squaring the sum; this term has to be added to account for the fact that the term $r = s = 0$ doesn't appear in the sum, because of $\gcd(0, 0, m) = m$.

terms add up to $\frac{\varphi(m)}{m^2}$ times the sum over the areas of the smaller rectangles, which is the area of the big rectangle. Hence,

$$\mathcal{N}_m(\mathcal{X} \times \mathcal{Y}) = \frac{\varphi(m)}{m^2} XY + O_\varepsilon\left(m^{\frac{1}{2}+\varepsilon}\left(1 + \frac{X}{m}\right)\left(1 + \frac{Y}{m}\right)\right). \quad (2.11)$$

2.2.2. Distribution in Regions bounded by a smooth Function

Since we now have sufficient control over the quantity $\mathcal{N}_m(\Omega)$ for rectangular regions Ω it is a standard idea from calculus to use Riemann sums to better understand $\mathcal{N}_m(\Omega)$ for a region Ω bounded from above and below by two sufficiently smooth functions. The following lemma due to Boca [2007] provides the details on this idea.

Lemma 2.2. Let $f \in C^1[\alpha, \beta]$ be a positive function. For

$$\Omega = \{(x, y) \in \mathbb{R}^2 \mid \alpha \leq x \leq \beta, 0 \leq y \leq f_2(x)\}$$

it holds that

$$\mathcal{N}_m(\Omega) = \frac{\varphi(m)}{m^2} \text{area}(\Omega) + \mathcal{E}_m$$

for every $T \in \mathbb{N}$, where \mathcal{E}_m obeys

$$\mathcal{E}_m \ll_\varepsilon \frac{\beta - \alpha}{Tm} V_\alpha^\beta(f) + Tm^{\frac{1}{2}+\varepsilon} \left(1 + \frac{\beta - \alpha}{Tm}\right) \left(1 + \frac{\|f\|_\infty}{m}\right).$$

PROOF: We partition $[\alpha, \beta]$ into T intervals $I_i = [\alpha_i, \beta_i]$ of equal size. Let

$$m_i := \min_{x \in I_i} f(x) \quad \text{and} \quad M_i := \max_{x \in I_i} f(x).$$

The inclusions

$$\bigcup_{i=1}^T (I_i \times [0, m_i]) \subseteq \Omega \subseteq \bigcup_{i=1}^T (I_i \times [0, M_i])$$

imply

$$\sum_{i=1}^T \mathcal{N}_m(I_i \times [0, m_i]) \leq \mathcal{N}_m(\Omega) \leq \sum_{i=1}^T \mathcal{N}_m(I_i \times [0, M_i]).$$

Using $m_i \leq \|f\|_\infty$ and applying (2.11) to the summands yields

$$\mathcal{N}_m(I_i \times [0, m_i]) = \frac{\varphi(m)}{m^2} \frac{\beta - \alpha}{T} m_i + O_\varepsilon(\mathcal{E}_T(m)),$$

with error term

$$\mathcal{E}_T(m) := m^{\frac{1}{2}+\varepsilon} \left(1 + \frac{\beta - \alpha}{Tm}\right) \left(1 + \frac{\|f\|_\infty}{m}\right).$$

Hence,

$$\frac{\varphi(m)}{m^2} \sum_{i=1}^T \frac{\beta - \alpha}{T} m_i + O_\varepsilon(T\mathcal{E}_T(m)) \leq \mathcal{N}_m(\Omega) \leq \frac{\varphi(m)}{m^2} \sum_{i=1}^T \frac{\beta - \alpha}{T} M_i + O_\varepsilon(T\mathcal{E}_T(m))$$

and by

$$\sum_{i=1}^T \frac{\beta - \alpha}{T} m_i + O\left(\frac{\beta - \alpha}{T} V_\alpha^\beta(f)\right) = \int_\alpha^\beta f(x) dx = \sum_{i=1}^T \frac{\beta - \alpha}{T} M_i + O\left(\frac{\beta - \alpha}{T} V_\alpha^\beta(f)\right)$$

and estimating $\frac{\varphi(m)}{m^2} \leq \frac{1}{m}$ we find that

$$\mathcal{N}_m(\Omega) - \frac{\varphi(m)}{m^2} \int_{\alpha}^{\beta} f(x) dx = O\left(\frac{\beta - \alpha}{Tm} V_{\alpha}^{\beta}(f) + T\mathcal{E}_T(m)\right). \quad \blacksquare$$

Notice, the larger one takes T the better the integral will be approximated by the corresponding Riemann sums, thereby reducing the approximation error

$$\frac{\beta}{Tm} V_{\alpha}^{\beta}(f). \quad (2.12)$$

However, this refinement comes at the cost of having to apply (2.11) more often, thereby worsening the accumulative error term

$$Tm^{\frac{1}{2}+\varepsilon} \left(1 + \frac{\beta - \alpha}{Tm}\right) \left(1 + \frac{\|f\|_{\infty}}{m}\right). \quad (2.13)$$

Conversely, by taking T to be small one may hope to improve (2.13).

Hence, in practice one has to choose T appropriately in order to balance out the contribution from the terms (2.12), (2.13).

2.3 Disproving an alleged Generalization

In his paper Shparlinski [2012] states Theorem 2.1 in a greater generality. Apart from the fact that he considers more general modular hyperbolas, i.e.

$$\mathcal{H}_{a,m} := \{(x, y) \in \mathbb{Z}^2 \mid xy \equiv a \pmod{m}\} \quad (2.14)$$

for $a \in \mathbb{Z}$ coprime to m he also allows the set \mathcal{Y} (see Theorem 2.1) to depend on $x \in \mathcal{X}$. The precise statement reads as follows [Shparlinski, 2012, Theorem 13]:

Let $\mathcal{X} = \{U + 1, \dots, U + X\}$, where $m > X \geq 1$ and $U \geq 0$ are arbitrary integers. Suppose that for every $x \in \mathcal{X}$ we are given a set $\mathcal{Y}_x = \{V_x + 1, \dots, V_x + Y\}$ where $m > Y \geq 1$ and $V_x \geq 0$ are arbitrary integers. Then for any integer $m \geq 1$ and a with $\gcd(a, m) = 1$, we have

$$\sum_{\substack{(x,y) \in \mathcal{H}_{a,m} \\ x \in \mathcal{X}, y \in \mathcal{Y}_x}} 1 = \frac{\varphi(m)}{m^2} XY + O(m^{\frac{1}{2}+o(1)}). \quad (2.15)$$

A minimal order of the function φ is given by

$$e^{-\gamma} \frac{n}{\log \log n},$$

that is,²

$$\liminf_{n \rightarrow \infty} \frac{\varphi(n) \log \log n}{n} = e^{-\gamma}.$$

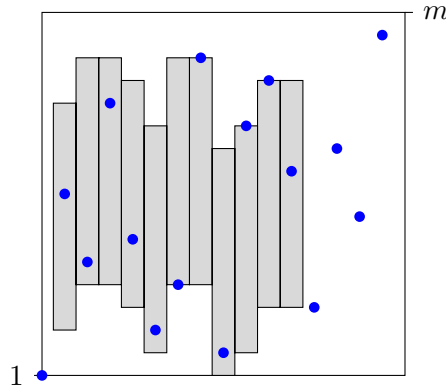
In particular one expects the main term (2.15) to be bigger than the error term whenever $|XY| \geq m^{\frac{3}{2}}$.

²see, for instance, Tenenbaum [1995].

For $a = 1$ the left hand side in (2.15) is precisely $\mathcal{N}_m(\Omega)$ for

$$\Omega = \bigcup_{x=1}^X [U+x] \times [V_x+1, V_x+Y],$$

where Ω may be thought of as a “disarranged rectangle”.



For a not necessarily equal to 1 one has an analogous interpretation after making the obvious adjustment to the definition of \mathcal{N}_m , i.e. replacing (2.1) in (2.2) with (2.14).

We would like to note, that the proof given for this statement (which we have reproduced as proof of Theorem 2.1) fails unless V_x is assumed to be independent of x . Indeed, going from (2.9) to (2.10) becomes impossible since the second sum in

$$\sum_{w=U+1}^{U+X} e_m(-rw) \sum_{z=V_w+1}^{V_w+Y} e_m(-sz)$$

depends on w .

In fact, not only the proof fails when working in this generality; we assume $m = p$ to be prime and let $\mathcal{X} = \{1, \dots, p-1\}$. Furthermore, we let $Y = 1$ and choose V_x appropriately in order to “catch” all hyperbola points, i.e. $\mathcal{Y}_x = \{\bar{x}\}$, where $\bar{x} \in [1, p)$ is the unique integer such that $(x, \bar{x}) \in \mathcal{H}_p$. We obtain

$$\sum_{\substack{(x,y) \in \mathcal{H}_{a,p} \\ x \in \mathcal{X}, y \in \mathcal{Y}_x}} 1 = \varphi(p) = p-1,$$

which according to the above statement is supposed to be equal to

$$\frac{(p-1)^2}{p^2} + O(p^{\frac{1}{2}+o(1)}) = O(p^{\frac{1}{2}+o(1)}),$$

an obvious contradiction.

Chapter 3

On the Quantity $\Psi(N)$, Boca's Paper

In Section §1.3 we have studied the distribution of numbers in the Calkin-Wilf tree associated with matrices of fixed trace n . The number $\mathbf{N}(n, m)$ of such numbers having integer part m was of particular interest to us. This chapter deals with the overall number $\Psi(N)$ of numbers in the Calkin-Wilf tree with associated trace at most N (but not equal to 2 since their number is infinite). That is,

$$\Psi(N) := \sum_{3 \leq n \leq N} \Phi(n),$$

where

$$\Phi(n) := \sum_{m=0}^{\infty} \mathbf{N}(n, m).$$

By Theorem 1.3, we may also write

$$\Phi(n) = \sum_{m=0}^{n-2} \mathbf{N}(n, m) = 2\mathbf{N}(n, 0)$$

This quantity was studied previously with theoretical physics in mind, see Boca [2007] and references therein. We do not pursue this aspect any further and look at the quantity $\Psi(N)$ entirely with its connection to the Calkin-Wilf tree in mind.

In this chapter we give an exposition of the paper [Boca, 2007] and correct some minor errors. The overall goal is to establish the asymptotic formula

$$\Psi(N) = c_1 N^2 \log N + c_2 N^2 + \mathcal{O}_\varepsilon(N^{\frac{7}{4}+\varepsilon}) \tag{3.1}$$

with constants¹

$$c_1 = \frac{1}{\zeta(2)}, \quad c_2 = \frac{1}{\zeta(2)} \left(\gamma - \frac{3}{2} - \frac{\zeta'(2)}{\zeta(2)} \right).$$

We try to give more details than Boca [2007] where we deem it necessary. Some arguments were changed slightly and expanded upon. On the other hand, we appeal to figures rather than formulas to illustrate some main ideas in the proofs. A reader who would rather see more formulas is warmly referred to the original paper by Boca, although, the formulas should be easily obtained from what can be found in this thesis.

¹Note, that Boca [2007, Theorem 1.1] gives an incorrect value for c_2 .

3.1 Reduction to Estimating a Number of Hyperbola Points

Using the notation from Section 1.2.2, we recall the formulas

$$R^{a_1} L^{a_2} \dots R^{a_{2m-1}} L^{a_{2m}} = \begin{pmatrix} q_{2m} & q_{2m-1} \\ p_{2m} & p_{2m-1} \end{pmatrix}, \quad (3.2)$$

$$L^{a_1} R^{a_2} \dots L^{a_{2m-1}} R^{a_{2m}} = \begin{pmatrix} p_{2m-1} & p_{2m} \\ q_{2m-1} & q_{2m} \end{pmatrix}, \quad (3.3)$$

$$R^{a_1} L^{a_2} \dots R^{a_{2m-1}} L^{a_{2m}} R^{a_{2m+1}} = \begin{pmatrix} q_{2m} & q_{2m+1} \\ p_{2m} & p_{2m+1} \end{pmatrix}, \quad (3.4)$$

$$L^{a_1} R^{a_2} \dots L^{a_{2m-1}} R^{a_{2m}} L^{a_{2m+1}} = \begin{pmatrix} p_{2m+1} & p_{2m} \\ q_{2m+1} & q_{2m} \end{pmatrix}. \quad (3.5)$$

Note, that the matrices in (3.2) and (3.3) as well as (3.4) and (3.5) have equal trace. Therefore, it suffices to consider products of L s and R s starting with R .

We let

$$\begin{aligned} \mathcal{W}_{\text{ev}}(N) &:= \{(a_1, \dots, a_{2m}) \in \mathbb{N}^{2m} \mid m \geq 1, \text{tr } R^{a_1} L^{a_2} \dots R^{a_{2m-1}} L^{a_{2m}} \leq N\}, \\ \mathcal{W}_{\text{odd}}(N) &:= \{(a_1, \dots, a_{2m+1}) \in \mathbb{N}^{2m+1} \mid m \geq 1, \text{tr } R^{a_1} L^{a_2} \dots R^{a_{2m-1}} L^{a_{2m}} R^{a_{2m+1}} \leq N\} \end{aligned}$$

and denote by $\Psi_{\text{ev}}(N)$ and $\Psi_{\text{odd}}(N)$ their respective cardinalities. By the previous remark we find

$$\Psi(N) = 2\Psi_{\text{ev}}(N) + 2\Psi_{\text{odd}}(N) \quad (3.6)$$

and we face the problem of estimating $\Psi_{\text{ev}}(N)$ and $\Psi_{\text{odd}}(N)$. We do this by looking at the possible values of (3.2) and (3.4). Let

$$\begin{aligned} \mathcal{S}_{\text{ev}}(N) &:= \left\{ \begin{pmatrix} q' & q \\ p' & p \end{pmatrix} \mid \begin{array}{l} 0 \leq p \leq q, \quad 0 \leq p' \leq q', \quad q' > q, \\ p + q' \leq N, \quad pq' - p'q = 1 \end{array} \right\}, \\ \mathcal{S}_{\text{odd}}(N) &:= \left\{ \begin{pmatrix} q & q' \\ p & p' \end{pmatrix} \mid \begin{array}{l} 0 \leq p \leq q, \quad 0 \leq p' \leq q', \quad q' \geq q, \\ p' + q \leq N, \quad p'q - pq' = 1 \end{array} \right\}. \end{aligned}$$

We have the obvious maps

$$\beta_{N,\text{ev}} : \mathcal{W}_{\text{ev}}(N) \longrightarrow \mathcal{S}_{\text{ev}}(N) \quad \text{and} \quad \beta_{N,\text{odd}} : \mathcal{W}_{\text{odd}}(N) \longrightarrow \mathcal{S}_{\text{odd}}(N),$$

both given by

$$(a_1, \dots, a_k) \longmapsto M(a_1) \cdots M(a_k)$$

(see (1.7)). As exploited many times in Chapter 1, the monoid \mathcal{M} generated by L and R is free over $\{L, R\}$, whence the maps $\beta_{N,\text{ev}}$ and $\beta_{N,\text{odd}}$ are injective.

In fact, they are also surjective: if given q_\bullet we can easily recover a_\bullet . Indeed, by (1.4),

$$\left\lfloor \frac{q_{n+1}}{q_n} \right\rfloor = a_{n+1} \quad (n \geq 1).$$

So, given

$$X = \begin{pmatrix} q' & q \\ p' & p \end{pmatrix} \in \mathcal{S}_{\text{ev}}(N) \quad (3.7)$$

and wishing to write $X = \beta_{N,\text{ev}}((a_{2m}, \dots, a_1))$ for some $(a_{2m}, \dots, a_1) \in \mathcal{W}_{\text{ev}}(N)$, it seems natural

to let $a_1 := \lfloor \frac{q'}{q} \rfloor$ and consider

$$X \cdot M(a_1)^{-1} = \begin{pmatrix} q' & q \\ p' & p \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & -a_1 \end{pmatrix} = \begin{pmatrix} q & q' - a_1 q \\ p & p' - a_1 p \end{pmatrix}.$$

Repeating this procedure with $(q, q' - a_1 q)$ replacing the part of (q', q) one is essentially mimicking Euclid's algorithm for determining the greatest common divisor of q' and q in the first row of the resulting matrices

$$X \cdot M(a_1)^{-1} \cdots M(a_k)^{-1}.$$

Because of $pq' - p'q = 1$ we have $\gcd(q, q') = 1$ and it follows that

$$X \cdot M(a_1)^{-1} \cdots M(a_k)^{-1} = \begin{pmatrix} 1 & 0 \\ b & c \end{pmatrix}, \quad (3.8)$$

for some $k \in \mathbb{N}$ and suitable $b, c \in \mathbb{Z}$.

Furthermore, for $q > 1$ we have

$$a_1 = \left\lfloor \frac{q'}{q} \right\rfloor \leq \frac{q'}{q} - \frac{1}{q} \leq \frac{q' - p'}{q - p}$$

and since

$$\frac{q' - p'}{q - p} - \frac{q' - 1}{q} = \frac{1 + q - p}{q - p} > 0$$

we conclude that

$$p' - a_1 p \leq q' - a_1 q$$

(note that this formula also holds in the case $q = 1$ since we have $p' - a_1 p = p'q - q'p = -1$; the case $q = 0$ does not occur). Applying this reasoning to a_2, a_3, \dots and looking at

$$X \cdot M(a_1)^{-1} \cdots M(a_{k-1})^{-1} = \begin{pmatrix} 1 & 0 \\ b & c \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & a_k \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ c & b + a_k c \end{pmatrix}$$

we find $b + a_k c \leq 1$ and hence $\{b, c\} = \{0, 1\}$. Using that (3.8) must have determinant ± 1 we find $(b, c) = (0, 1)$ and thus

$$X = M(a_1) \cdots M(a_k);$$

in particular, $k = 2m$ must be even, as seen by taking determinants in the above equation. This proves that $\beta_{N,\text{ev}}$ is surjective. One argues similarly for $\beta_{N,\text{odd}}$.

3.1.1. Words of Even Length

Next, we parametrize the set $\mathcal{S}_{\text{ev}}(N)$. Consider X as in (3.7). Previously, we have seen that q and q' are coprime and

$$pq' - p'q = 1 \quad (3.9)$$

implies $pq' \equiv 1 \pmod{q}$, which by $p \leq q$ gives $p = \bar{q}'$, where $\bar{q}' \in \{1, \dots, q\}$ is the inverse of q' modulo q . Furthermore, (3.9) yields

$$p' = \frac{pq' - 1}{q} \leq \frac{qq' - 1}{q} < q'.$$

Consequently, the map

$$\{(q, q') \mid q < q' \leq N, \gcd(q, q') = 1, q' + \bar{q}' \leq N\} \longrightarrow \mathcal{S}_{\text{ev}}(N)$$

given by

$$(q, q') \mapsto \begin{pmatrix} q' & q \\ \frac{\bar{q}q'-1}{q} & q' \end{pmatrix}$$

is bijective. From this we infer

$$|\Psi_{\text{ev}}(N)| = |\mathcal{S}_{\text{ev}}(N)| = \sum_{\substack{q < q' \leq N \\ \gcd(q, q') = 1 \\ q' + q \leq N}} 1 = \sum_{m < N} \sum_{\substack{m < y \leq N \\ 0 < x \leq \min\{m, N-y\} \\ xy \equiv 1 \pmod{m}}} 1. \quad (3.10)$$

3.1.2. Words of Odd Length

As done previously to $\mathcal{S}_{\text{ev}}(N)$ we now seek to estimate $\mathcal{S}_{\text{odd}}(N)$. To this end, for x coprime to p we redefine \bar{x} to mean the integer in $\{1, \dots, p\}$ inverse to x modulo p (note, that in comparison to the definition of \bar{x} from section 3.1.1 only q was changed to p).

We start by looking at the equation

$$p'q - pq' = 1. \quad (3.11)$$

By solving for p' and multiplying by q we find

$$qp' = pq' + 1 \quad \text{and} \quad qp' \equiv 1 \pmod{p}.$$

Therefore, $p' \equiv \bar{q} \pmod{p}$ and hence

$$p' = \bar{q} + pt \quad (3.12)$$

for some $t \in \mathbb{Z}$. The inequality $p' + q \leq N$ imposes the restriction

$$t \leq \left\lfloor \frac{N - q - \bar{q}}{p} \right\rfloor$$

on t . Since $p \geq p'$ would imply

$$0 \geq p(q - q') = pq - pq' \geq p'q - pq' = 1,$$

a contradiction, we must have $p < p'$ and in combination with (3.12) we deduce the additional restriction $t \geq 1$.

Solving (3.11) for q' yields

$$q' = \frac{p'q - 1}{p} = \frac{\bar{q}q - 1}{p} + qt.$$

We conclude that $\mathcal{S}_{\text{odd}}(N)$ may be parametrized by (q, p, t) subject to the above conditions (obviously each choice for t within the afore obtained bounds is admissible), i.e. the map

$$\left\{ (q, p, t) \mid 0 \leq p < q, \gcd(p, q) = 1, 1 \leq t \leq \left\lfloor \frac{N - q - \bar{q}}{p} \right\rfloor \right\} \longrightarrow \mathcal{S}_{\text{odd}}(N)$$

given by

$$(q, p, t) \mapsto \begin{pmatrix} q & \frac{\bar{q}q-1}{p} + qt \\ p & \bar{q} + pt \end{pmatrix}$$

is bijective.

As a consequence we have

$$\Psi_{\text{odd}}(N) = \sum_{q < N} \sum_{\substack{p < q \\ \gcd(p,q)=1 \\ q+\bar{q} \leq N}} \left\lfloor \frac{N - q - \bar{q}}{p} \right\rfloor = \sum_{m < N} \sum_{\substack{m < y < N \\ 0 < x \leq \min\{m, N-y\} \\ xy \equiv 1 \pmod{m}}} \left\lfloor \frac{N - x - y}{m} \right\rfloor.$$

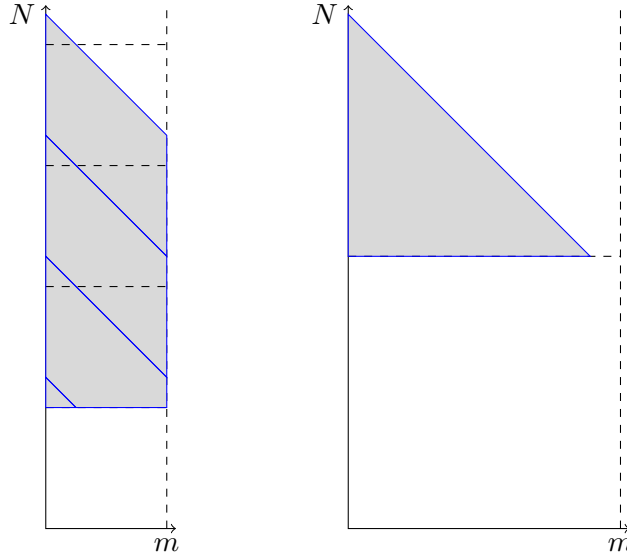
The formula amounts to counting points $(x, y) \in \mathcal{H}_m$ within the region

$$\Omega_{N,m} := \{(x, y) \in \mathbb{R}^2 \mid m < y < N, 0 < x \leq \min\{m, N - y\}\}$$

with respect to the weight function

$$w_{N,m} : (x, y) \mapsto \left\lfloor \frac{N - x - y}{m} \right\rfloor. \quad (3.13)$$

For $m < \frac{N}{2}$ this region takes the form of a trapezoid and for $m \geq \frac{N}{2}$ it degenerates into a triangle, as visualized by the following figure:



We continue by decomposing Ω into sets on which the weight $w_{N,m} = i$ is constant ($i = 0, 1, \dots$). The sets $\Omega_{N,m,i} := w_{N,m}^{-1}(i) \cap \Omega_{N,m}$ are given by

$$\Omega_{N,m,i} = \{(x, y) \in (0, m] \times (m, N - m) \mid N - (i + 1)m < x + y \leq N - im\}; \quad (3.14)$$

these are drawn as regions bounded by blue lines in the above figure. Since for $m \geq \frac{N}{2}$ the region $\Omega_{N,m,0}$ of weight 0 coincides with Ω ,

$$\Psi_{\text{odd}}(N) = \sum_{m < \frac{N}{2}} \sum_{i=1}^{\lfloor \frac{N}{m} \rfloor - 1} i \mathcal{N}_m(\Omega_{N,m,i}).$$

Now, we intend to write

$$\Psi_{\text{odd}}(N) = \sum_{m < \frac{N}{2}} \mathcal{N}_m(\mathcal{T}_{N,m}) \quad (3.15)$$

for suitable regions $\mathcal{T}_{N,m} \subseteq \mathbb{R}^2$, thereby encoding the weighting process into the region. To achieve this, note that

$$\mathcal{N}_m(\Omega') = \mathcal{N}_m(v + \Omega') \quad (3.16)$$

holds for any region $\Omega' \subseteq \mathbb{R}^2$ and any vector $v \in m\mathbb{Z}^2$. Therefore, for each summand $i\mathcal{N}_m(\Omega_{N,m,i})$ we have

$$i\mathcal{N}_m(\Omega_{N,m,i}) = \mathcal{N}_m(\Omega'_{N,m,i}),$$

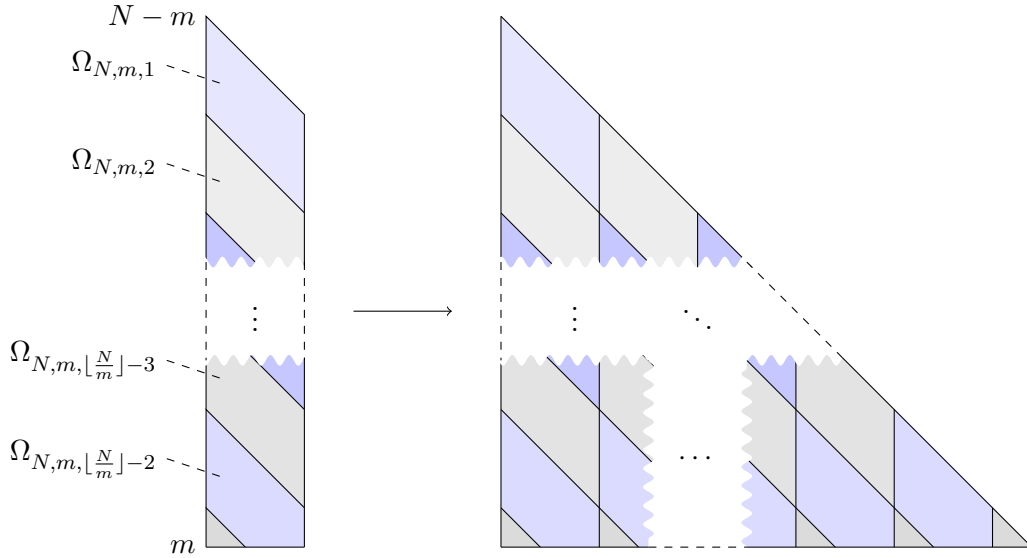
where

$$\Omega'_{N,m,i} := \bigcup_{j=0}^{i-1} ((jm, 0) + \Omega_{N,m,i}).$$

Consequently, (3.15) holds if we let

$$\mathcal{T}_{N,m} := (0, -m) + \bigcup_{i=1}^{\lfloor \frac{N}{m} \rfloor - 1} \Omega'_{N,m,i} = \{(x, y) \in \mathbb{R}^2 \mid 0 < x \leq N - 2m, 0 < y \leq N - 2m - x\}. \quad (3.17)$$

The procedure of going from $\Omega_{N,m,i}$ to $\Omega'_{N,m,i}$ may be visualized as putting i pieces in the shape of $\Omega_{N,m,i}$ next to each other (see the figure below). Fitting the resulting shapes together one obtains $(0, m) + \mathcal{T}_{N,m}$, a triangle.



3.2 Estimating $\Psi_{\text{ev}}(N)$ and $\Psi_{\text{odd}}(N)$

3.2.1. Words of Even Length

We shall now return to considering $\Psi_{\text{ev}}(N)$. Let

$$\begin{aligned} \Omega_{\text{ev},m} &:= \{(x, y) \in \mathbb{R}^2 \mid 0 < x \leq m < y \leq N\}, \\ \Omega'_{\text{ev},m} &:= \{(x, y) \in \mathbb{R}^2 \mid m < y \leq N, 0 < x \leq N - y\}. \end{aligned}$$

Using the regions $\Omega_{\text{ev},m}$ and $\Omega'_{\text{ev},m}$ we recover $\mathcal{N}_m(\Omega_{\text{ev},m})$ and $\mathcal{N}_m(\Omega'_{\text{ev},m})$ in (3.10). More precisely,

$$\Psi_{\text{ev}}(N) = \sum_{m < \frac{N}{2}} \mathcal{N}_m(\Omega_{\text{ev},m}) + \sum_{\frac{N}{2} \leq m \leq N} \mathcal{N}_m(\Omega'_{\text{ev},m}),$$

By appealing to (3.16) and applying Lemma 2.2 to the translated regions $(0, -m) + \Omega_{\text{ev},m}$,

$(0, -m) + \Omega'_{\text{ev},m}$ we arrive at

$$\begin{aligned}\mathcal{N}_m(\Omega_{\text{ev},m}) &= \frac{\varphi(m)}{m^2} \frac{m(2N-3m)}{2} + \mathcal{E}_m(N), \\ \mathcal{N}_m(\Omega'_{\text{ev},m}) &= \frac{\varphi(m)}{m^2} \frac{(N-m)^2}{2} + \mathcal{E}'_m(N)\end{aligned}$$

with error terms

$$\mathcal{E}_m(N) \ll_{\varepsilon} \frac{m}{T} + m^{-\frac{1}{2}+\varepsilon} N(T+1) \ll_{\varepsilon} \frac{m}{T} + m^{-\frac{1}{2}+\varepsilon} NT, \quad (3.18)$$

$$\mathcal{E}'_m(N) \ll_{\varepsilon} \frac{(N-m)^2}{Tm} + m^{\frac{1}{2}+\varepsilon} \left(T-1 + \frac{N}{m}\right) \frac{N}{m} \ll_{\varepsilon} \frac{(N-m)^2}{Tm} + m^{\frac{1}{2}+\varepsilon} \left(T + \frac{N}{m}\right) \frac{N}{m}, \quad (3.19)$$

where $T \in \mathbb{N}$ can be chosen arbitrarily.

By expanding the expressions in (2.12) and (2.13) and appealing to monotonicity of the resulting summands we can bound the resulting sums by corresponding integrals and find that

$$\sum_{m < \frac{N}{2}} \mathcal{E}_m(N) + \sum_{\frac{N}{2} \leq m \leq N} \mathcal{E}'_m(N) \ll_{\varepsilon} N^{\frac{7}{4}+\varepsilon},$$

when choosing T to be $\lfloor N^{\frac{1}{4}} \rfloor$. This implies

$$\Psi_{\text{ev}}(N) = \sum_{m < \frac{N}{2}} \frac{\varphi(m)}{m^2} \frac{m(2N-3m)}{2} + \sum_{\frac{N}{2} \leq m \leq N} \frac{\varphi(m)}{m^2} \frac{(N-m)^2}{2} + O_{\varepsilon}(N^{\frac{7}{4}+\varepsilon}).$$

3.2.2. Words of Odd Length, $\sqrt{N} < m$

Our next objective is to apply similar reasoning to $\Psi_{\text{odd}}(N)$. Since the (first) projection

$$\text{pr}_1 \mathcal{T}_{N,m} := \{x \in \mathbb{R} \mid \exists y : (x, y) \in \mathcal{T}_{N,m}\} = (0, N-2m]$$

of $\mathcal{T}_{N,m}$ from (3.17) is much bigger (length-wise) than $\text{pr}_1 \Omega_{\text{ev},m}$ the size of the quantity $\beta - \alpha$ from Lemma 2.2 becomes problematic. Indeed, if applying Lemma 2.2 naively to (3.15) we obtain

$$\Psi_{\text{odd}}(N) = \sum_{m < \frac{N}{2}} \left(\frac{\varphi(m)}{m^2} \frac{(N-2m)^2}{2} + \mathcal{E}''_m \right)$$

with error term

$$\mathcal{E}''_m \ll_{\varepsilon} \frac{N-2m}{Tm} (N-2m) + Tm^{\frac{1}{2}+\varepsilon} \left(1 + \frac{N-2m}{Tm}\right) \frac{N-m}{m}. \quad (3.20)$$

Even just summing over the last term yields

$$\begin{aligned}\sum_{m < \frac{N}{2}} Tm^{\frac{1}{2}+\varepsilon} \frac{N-2m}{Tm} \frac{N-m}{m} &\geq \sum_{m < \frac{N}{2}} m^{-\frac{1}{2}+\varepsilon} (N-2m)^2 \\ &\geq \int_1^{\frac{N}{2}} x^{-\frac{1}{2}+\varepsilon} (N-2x)^2 dx \geq N^{\frac{5}{2}+\varepsilon},\end{aligned} \quad (3.21)$$

which is still bigger than the expected main term (see (3.1)).

We will circumvent this problem by further decomposing $\mathcal{T}_{N,m}$ for small m . Note, that the biggest contribution to the integral in (3.21) comes from values attained by the integral kernel at small arguments. For big m , that is $\sqrt{N} < m < \frac{N}{2}$, we still use the crude estimate (3.20) to

obtain

$$\mathcal{E}_m'' \ll_{\varepsilon} \frac{N^2}{Tm} + TNm^{-\frac{1}{2}+\varepsilon} + N^2m^{-\frac{3}{2}+\varepsilon}.$$

The sum over this expression is again easily estimated by comparison with the corresponding integrals,

$$\begin{aligned} \sum_{N^c < m < \frac{N}{2}} \mathcal{E}_m'' &\ll_{\varepsilon} \sum_{\sqrt{N} < m < \frac{N}{2}} \left(\frac{N^2}{Tm} + TNm^{-\frac{1}{2}+\varepsilon} + N^2m^{-\frac{3}{2}+\varepsilon} \right) \\ &\ll_{\varepsilon} \frac{N^2}{T} \sum_{\sqrt{N} < m < \frac{N}{2}} \frac{1}{m} + TN \sum_{\sqrt{N} < m < \frac{N}{2}} m^{-\frac{1}{2}+\varepsilon} + N^2 \sum_{\sqrt{N} < m < \frac{N}{2}} m^{-\frac{3}{2}+\varepsilon} \\ &\ll_{\varepsilon} \frac{N^2}{T} \log N + TN^{1+\frac{1}{2}} + N^{2-\frac{1}{4}+\frac{1}{2}\varepsilon}. \end{aligned}$$

The usual choice $T = \lfloor N^{\frac{1}{4}} \rfloor$ yields

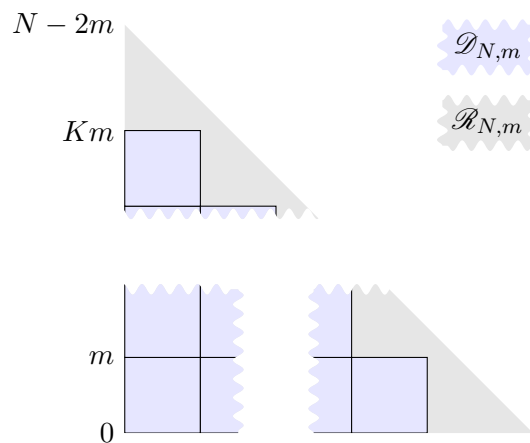
$$\sum_{\sqrt{N} < m < \frac{N}{2}} \mathcal{N}_m(\mathcal{T}_{N,m}) = \sum_{\sqrt{N} < m < \frac{N}{2}} \frac{\varphi(m)}{m^2} \frac{(N-2m)^2}{2} + O_{\varepsilon}(N^{\frac{7}{4}+\varepsilon}). \quad (3.22)$$

3.2.3. Words of Odd Length, $m \leq \sqrt{N}$

Now, we deal with small m , i.e. $m \leq \sqrt{N}$. Let $K := \lfloor \frac{N}{m} \rfloor - 3$.² For N sufficiently large we have $\sqrt{N} < \frac{N}{3}$ and K will be non-negative. The triangle $\mathcal{T}_{N,m}$ contains the union

$$\mathcal{D}_{N,m} := \bigcup_{i=1}^K \bigcup_{j=1}^{K-i+1} ((i-1)m, im] \times ((j-1)m, jm]$$

of $K + (K-1) + \dots + 1 = \frac{K(K+1)}{2}$ squares of side length m . The remaining part $\mathcal{T}_{N,m} \setminus \mathcal{D}_{N,m}$ of $\mathcal{T}_{N,m}$ will be called $\mathcal{R}_{N,m}$.



Since there are precisely $\varphi(m)$ points from \mathcal{H}_m in the squares we have

$$\mathcal{N}_m(\mathcal{D}_{N,m}) = \frac{K(K+1)}{2} \varphi(m) = \frac{\varphi(m)}{m^2} \text{area}(\mathcal{D}_{N,m}). \quad (3.23)$$

²Note, that in [Boca, 2007, proof of Lemma 4.1] there is a typo. Therein it reads $K = \lfloor \frac{N}{m} \rfloor - 2$, but this is too big.

The residual region $\mathcal{R}_{N,m}$ consists of K trapezoids and/or triangles each contained in a translation of the rectangle

$$(0, m] \times (0, 2m]$$

and one trapezoid/triangle contained in a translation of the rectangle

$$(0, 2m] \times (0, m].$$

Therefore,³

$$\mathcal{N}_m(\mathcal{R}_{N,m}) \leq 2(K+1)\varphi(m) < 2 \left\lfloor \frac{N}{m} \right\rfloor \varphi(m) \leq 2N$$

and consequently,

$$\sum_{m \leq \sqrt{N}} \mathcal{N}_m(\mathcal{R}_{N,m}) < 2N^{1+\frac{1}{2}}. \quad (3.24)$$

Furthermore,

$$\begin{aligned} \sum_{m \leq \sqrt{N}} \frac{\varphi(m)}{m^2} \text{area}(\mathcal{R}_{N,m}) &\leq \sum_{m \leq \sqrt{N}} \frac{1}{m} \text{area}(\mathcal{R}_{N,m}) \leq \sum_{m \leq \sqrt{N}} \frac{2m^2(K+1)}{m} \\ &\leq \sum_{m \leq \sqrt{N}} \frac{2m^2}{m} \frac{N}{m} \leq 2N^{1+\frac{1}{2}}. \end{aligned} \quad (3.25)$$

By virtue of (3.23), (3.24) and (3.25),

$$\begin{aligned} \sum_{m \leq \sqrt{N}} \mathcal{N}_m(\mathcal{T}_{N,m}) &= \sum_{m \leq \sqrt{N}} \mathcal{N}_m(\mathcal{D}_{N,m}) + O(N^{1+\frac{1}{2}}) \\ &= \sum_{m \leq \sqrt{N}} \frac{\varphi(m)}{m^2} \text{area}(\mathcal{D}_{N,m}) + O(N^{1+\frac{1}{2}}) \\ &= \sum_{m \leq \sqrt{N}} \frac{\varphi(m)}{m^2} (\text{area}(\mathcal{T}_{N,m}) - \text{area}(\mathcal{R}_{N,m})) + O(N^{1+\frac{1}{2}}) \\ &= \sum_{m \leq \sqrt{N}} \frac{\varphi(m)}{m^2} \text{area}(\mathcal{T}_{N,m}) + O(N^{1+\frac{1}{2}}) \\ &= \sum_{m \leq \sqrt{N}} \frac{\varphi(m)}{m^2} \frac{(N-2m)^2}{2} + O(N^{\frac{3}{2}}). \end{aligned} \quad (3.26)$$

Now, looking at (3.15), (3.26) and (3.22) we conclude that

$$\Psi_{\text{odd}}(N) = \sum_{m < \frac{N}{2}} \frac{\varphi(m)}{m^2} \frac{(N-2m)^2}{2} + O_\varepsilon(N^{\frac{7}{4}+\varepsilon}). \quad (3.27)$$

3.3 Finding an Analytic Expression for the Main Terms

After proving (3.27) Boca [2007] gives a detailed proof of the formula

$$\sum_{m < \frac{N}{2}} \frac{\varphi(m)}{m^2} \frac{(N-2m)^2}{2} = \frac{N^2}{2\zeta(2)} \left(\log N + \gamma - \log 2 - \frac{3}{2} - \frac{\zeta'(2)}{\zeta(2)} \right) + O(N), \quad (3.28)$$

³In [Boca, 2007, proof of Lemma 4.1] the factor 2 seems to be missing. However, examples like $(N, m) = (11, 4)$ show that the factor 2 cannot be replaced by 1.

thereby obtaining

$$\Psi_{\text{odd}}(N) = \frac{N^2}{2\zeta(2)} \left(\log N + \gamma - \log 2 - \frac{3}{2} - \frac{\zeta'(2)}{\zeta(2)} \right) + O_\varepsilon(N^{\frac{7}{4}+\varepsilon}) \quad (3.29)$$

from (3.27). Using this and known formulas for

$$\sum_{m < N} \varphi(m) \quad \text{and} \quad \sum_{m < N} \frac{\varphi(m)}{m}$$

he finds that

$$\sum_{m < N} \frac{\varphi(m)}{m^2} = \frac{1}{\zeta(2)} \left(\log N + \gamma - \frac{\zeta'(2)}{\zeta(2)} \right) + O\left(\frac{\log N}{N}\right).$$

By combining these formulas a straightforward calculation in (3.10) gives a formula for $\Psi_{\text{ev}}(N)$ similar to (3.29),

$$\Psi_{\text{ev}}(N) = \frac{N^2}{2\zeta(2)} \log 2 + O_\varepsilon(N^{\frac{7}{4}+\varepsilon}).$$

Together with (3.6) this proves (3.1).

We choose to deviate slightly from this path. Instead of dealing with the rather odd sum (3.28) we combine (3.6) with (3.27) and (3.10) and obtain the beautiful formula

$$\Psi(N) = \sum_{m < N} \frac{\varphi(m)}{m^2} (N - m)^2 + O_\varepsilon(N^{\frac{7}{4}+\varepsilon}). \quad (3.30)$$

Treating $\Psi(N)$ instead of treating $\Psi_{\text{ev}}(N)$ and $\Psi_{\text{odd}}(N)$ separately seems more natural since it is $\Psi(N)$ that we are interested in. Admittedly, apart from this there seem to be no other merits from the one approach over the other. The arguments that follow are still largely those found in [Boca, 2007].

We now seek to estimate

$$\sum_{m < N} \frac{\varphi(m)}{m^2} (N - m)^2.$$

Key ingredients for this task are Perron's formula and properties of the Riemann zeta-function. The reader unfamiliar with these concepts may find the most important cornerstones collected in appendix A.

We start by observing that by means of partial fraction decomposition one has

$$\frac{1}{s(s+1)(s+2)} = \frac{1}{2s} - \frac{1}{s+1} + \frac{1}{2(s+2)}. \quad (3.31)$$

Furthermore, let

$$f(s, y) := \frac{y^s}{s(s+1)(s+2)} \quad \text{and} \quad g(s) := 2N^2 \frac{\zeta(s+1)}{\zeta(s+2)} f(s, N).$$

Applying (A.1) to (3.31) gives

$$\frac{1}{2\pi i} \int_{\sigma_0 - i\infty}^{\sigma_0 + i\infty} f(s, y) ds = \begin{cases} 0, & 0 < s \leq 1, \\ \frac{1}{2} \left(1 - \frac{1}{y}\right)^2, & s > 1. \end{cases}$$

This identity can now be used to select the terms $m < N$ from (A.2) and add the weight $(N - m)$

to each such term. Indeed, using (A.2) we obtain

$$\begin{aligned}
 \frac{1}{2\pi i} \int_{\sigma_0 - i\infty}^{\sigma_0 + i\infty} g(s) ds &= \frac{N^2}{\pi i} \int_{\sigma_0 - i\infty}^{\sigma_0 + i\infty} \sum_{m=1}^{\infty} \frac{\varphi(m)}{m^{s+2}} f(s, N) ds \\
 &= \sum_{m=1}^{\infty} \frac{N^2 \varphi(m)}{m^2} \frac{1}{\pi i} \int_{\sigma_0 - i\infty}^{\sigma_0 + i\infty} f(s, N/m) ds \\
 &= \sum_{m < N} \frac{\varphi(m)}{m^2} (N - m)^2.
 \end{aligned} \tag{3.32}$$

The Laurent expansion (A.4) of ζ at 1 shows

$$g(s) = \left(\frac{1}{s^2} + \frac{\gamma}{s} + O(1) \right) \frac{1}{(s+2)\zeta(s+2)} \frac{2N^{s+2}}{s+1} \quad (s \rightarrow 0). \tag{3.33}$$

Furthermore, since the (simple) zero of $s \mapsto \frac{1}{\zeta(s+2)}$ at -1 cancels with the simple pole of $s \mapsto \frac{1}{s+1}$, we find that g admits a holomorphic extension to the region $\{s \in \mathbb{C} \mid \operatorname{Re} s > -2\}$ with the exception of the point $s = 0$, where g has a pole.

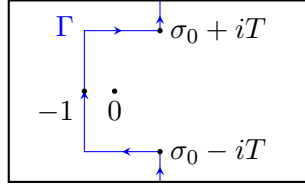
The function hiding behind the $O(1)$ -term in (3.33) is holomorphic. Therefore, the residue $\operatorname{res}_0 g$ of g at 0 is equal to the residue of

$$h : s \mapsto \frac{1 + s\gamma}{s^2(s+2)\zeta(s+2)} \frac{2N^{s+2}}{s+1}$$

at 0,

$$\operatorname{res}_0 g = \lim_{s \rightarrow 0} s^2 h(s) = \frac{N^2}{\zeta(2)} \left(\log N + \gamma - \frac{3}{2} - \frac{\zeta'(2)}{\zeta(2)} \right).$$

Now, for $T > 0$ we change the path of integration in (3.32) from $\sigma_0 + i\mathbb{R}$ to the contour Γ indicated in the following figure:



The residue theorem gives

$$\frac{1}{2\pi i} \int_{\sigma_0 - i\infty}^{\sigma_0 + i\infty} g(s) ds = \operatorname{res}_0 g + \frac{1}{2\pi i} \int_{\Gamma} g(s) ds. \tag{3.34}$$

In what follows we intend to show that the integral on the right hand side is small, provided T being sufficiently large. Indeed, by $|g(\sigma + it)| = |g(\sigma - it)|$ we have

$$\left| \int_{\Gamma} g(s) ds \right| \leq 2 \int_0^T |g(-1 + it)| dt + 2 \int_{-1}^{\sigma_0} |g(\sigma + iT)| d\sigma + 2 \int_T^{\infty} |g(\sigma_0 + it)| dt. \tag{3.35}$$

By virtue of (A.2),

$$\left| \frac{\zeta(\sigma_0 + 1 + it)}{\zeta(\sigma_0 + 2 + it)} \right| \leq \sum_{m=1}^{\infty} \frac{\varphi(m)}{m^{\sigma_0+2}} \leq \sum_{m=1}^{\infty} \frac{1}{m^{\sigma_0+1}} = \zeta(\sigma_0 + 1).$$

This enables us to estimate the last integral in (3.35),

$$\begin{aligned} \int_T^\infty |g(\sigma_0 + it)| dt &\ll_{\sigma_0} \int_T^\infty \left| \frac{\zeta(\sigma_0 + 1 + it)}{\zeta(\sigma_0 + 2 + it)} \right| \frac{N^{\sigma_0+2}}{t^3} dt \\ &\ll_{\sigma_0} N^{\sigma_0+2} \zeta(\sigma_0 + 1) \int_T^\infty \frac{1}{t^3} dt \ll_{\sigma_0} \frac{N^{\sigma_0+2}}{T^2}. \end{aligned} \quad (3.36)$$

We now use the estimates (A.8), (A.9). These imply

$$\int_{-1}^{\sigma_0} |g(\sigma + iT)| d\sigma \ll \frac{N^{\sigma_0+2}}{T^3} \int_{-1}^{\sigma_0} \left| \frac{\zeta(\sigma + 1 + iT)}{\zeta(\sigma + 2 + iT)} \right| d\sigma \ll_{\sigma_0, \varepsilon} \frac{N^{\sigma_0+2}}{T^3} T^{1+\varepsilon} \quad (3.37)$$

To estimate

$$\int_0^T |g(-1 + it)| dt$$

we use the functional equation (A.3) along with (A.7),

$$\frac{\zeta(it)}{\zeta(1+it)} = \chi(it) \frac{\zeta(1-it)}{\zeta(1+it)}, \quad \chi(s) = \frac{(2\pi)^s}{2\Gamma(s) \cos(\frac{\pi s}{2})},$$

and

$$|\Gamma(it)|^2 = \frac{\pi}{t \sinh(\pi t)}.$$

Because of $\zeta(\bar{s}) = \overline{\zeta(s)}$ and (A.10) we have

$$\left| \frac{\zeta(it)}{\zeta(1+it)} \right| = |\chi(it)| = \frac{1}{2\sqrt{\frac{\pi}{t \sinh(\pi t)} \cos(\frac{\pi t}{2}i)}} = \frac{\sqrt{t \sinh(\pi t)}}{2\sqrt{\pi} \cosh(\frac{\pi t}{2})} = \sqrt{\frac{t \tanh(\frac{\pi t}{2})}{2\pi}}.$$

Using⁴ (A.11) we obtain

$$\begin{aligned} \int_0^T |g(-1 + it)| dt &\ll N \left\{ \int_0^{\frac{2}{\pi}} + \int_{\frac{2}{\pi}}^T \right\} \left| \frac{\zeta(it)}{\zeta(1+it)} \right| \frac{1}{t(t^2+1)} dt \\ &\ll N \int_0^\infty \frac{1}{t^2+1} dt \ll N. \end{aligned} \quad (3.38)$$

Now let $T = N^2$ and $\sigma_0 = 1$. Combining (3.36), (3.37) and (3.38) in (3.35) yields

$$\frac{1}{2\pi i} \int_\Gamma g(s) ds \ll N.$$

By (3.34),

$$\sum_{m < N} \frac{\varphi(m)}{m^2} (N-m)^2 = \frac{N^2}{\zeta(2)} \left(\log N + \gamma - \frac{3}{2} - \frac{\zeta'(2)}{\zeta(2)} \right) + O(N)$$

and consequently it follows that

$$\Psi(N) = \frac{N^2}{\zeta(2)} \left(\log N + \gamma - \frac{3}{2} - \frac{\zeta'(2)}{\zeta(2)} \right) + O_\varepsilon(N^{\frac{7}{4}+\varepsilon}),$$

thereby proving (3.1).

⁴Boca [2007] writes $\tanh t \leq \max\{t, 1\}$ which obviously is correct as well. However, if using this estimate instead of (A.11) the integral $\int_0^{\frac{2}{\pi}} \dots$ fails to converge, because the pole at 0 of the integrand is not canceled.

Appendix A

Tools from Analysis

The present chapter arose from the discussion in section §3.3. The author of the thesis felt a particular discomfort in just using the needed tools ad hoc, so these tools have found their own place within this chapter. Although this doesn't change the fact that these are presented herein only with section §3.3 in mind and (mostly) without proof, putting them here, hopefully, makes the exposition clearer.

A.1 The Riemann Zeta-function

A.1.1. Some Identities and the Functional Equation

We start by giving a special case of Perron's formula (see e.g. Brüdern [1995, Lemma 1.4.1]). For $\sigma_0, y > 0$ one has

$$\frac{1}{2\pi i} \int_{\sigma_0 - i\infty}^{\sigma_0 + i\infty} \frac{y^s}{s} ds = \begin{cases} 0, & 0 < y < 1, \\ \frac{1}{2}, & y = 1, \\ 1, & y > 1, \end{cases} \quad (\text{A.1})$$

where the integral is understood in the Cauchy principal value sense. This formula is connected through the Mellin transform with the theory of Dirichlet series.

Next, we consider the Riemann zeta-function ζ given by

$$\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s} \quad \text{for} \quad \text{Re } s > 1.$$

From the Euler product

$$\zeta(s) = \prod_{p \in \mathbb{P}} (1 - p^{-s})^{-1}$$

one may deduce interesting formulas, among these,

$$\sum_{m=1}^{\infty} \frac{\varphi(m)}{m^s} = \frac{\zeta(s-1)}{\zeta(s)} \quad (\text{Re } s > 2); \quad (\text{A.2})$$

see Iwaniec and Kowalski [2004] or Brüdern [1995] for details.

By means of the functional equation [Titchmarsh, 2007, p.16]

$$\zeta(s) = \chi(s)\zeta(1-s),$$

where

$$\chi(s) = \pi^{s-\frac{1}{2}} \frac{\Gamma(\frac{1}{2} - \frac{1}{2}s)}{\Gamma(\frac{1}{2}s)}, \quad (\text{A.3})$$

one may define $\zeta(s)$ for $\operatorname{Re} s \leq 1$, $s \neq 1$, thereby obtaining a function holomorphic in $\mathbb{C} \setminus \{1\}$. At 1 the function ζ admits a pole of order 1 with residue 1. Moreover, we have the Laurent expansion [Titchmarsh, 2007, p.16]

$$\zeta(s) = \frac{1}{s-1} + \gamma + O(|s-1|). \quad (\text{A.4})$$

We also need a different expression for $\chi(s)$. Recall Legendres duplication formula

$$\Gamma(s)\Gamma\left(s + \frac{1}{2}\right) = 2^{1-2s}\pi^{\frac{1}{2}}\Gamma(2s). \quad (\text{A.5})$$

for the Gamma function and the reflection formula

$$\Gamma(s)\Gamma(1-s) = \frac{\pi}{\sin(\pi s)}. \quad (\text{A.6})$$

By (A.5),

$$\Gamma\left(\frac{1}{2}s\right)\Gamma\left(\frac{1}{2}s + \frac{1}{2}\right) = 2^{1-s}\pi^{\frac{1}{2}}\Gamma(s).$$

Putting $\frac{1}{2}s + \frac{1}{2}$ into (A.6) instead of s yields

$$\frac{\Gamma\left(\frac{1}{2} - \frac{1}{2}s\right)}{\Gamma\left(\frac{1}{2}s\right)} = \frac{2^s\pi^{\frac{1}{2}}}{2\Gamma(s)\cos\left(\frac{\pi}{2}s\right)}$$

and in combination with the previous formula we have

$$\chi(s) = \frac{(2\pi)^s}{2\Gamma(s)\cos\left(\frac{\pi}{2}s\right)}. \quad (\text{A.7})$$

A.1.2. Growth Estimates

In what follows, we use the standard notation $\sigma = \operatorname{Re} s$ and $t = \operatorname{Im} s$. For $\sigma > 1$ we have [Titchmarsh, 2007, p.51]

$$\frac{1}{\zeta(s)} = O((\log T)^7). \quad (\text{A.8})$$

Furthermore, for $\sigma \geq 0$, [Titchmarsh, 2007, p.69]

$$\zeta(s) \ll T \log T \ll_{\varepsilon} T^{1+\varepsilon}, \quad (\text{A.9})$$

where $T = |t| + 2$. Better estimates than (A.9) are known. However, these do not immediately improve upon the overall error term in Section §3.3 and are consequently omitted in favor of estimates whose proofs require less effort.

A.2 Hyperbolic Functions

We recall the standard definitions

$$\sinh s := \frac{e^s - e^{-s}}{2} \quad \text{and} \quad \cosh s := \frac{e^s + e^{-s}}{2},$$

as well as

$$\tanh s := \frac{\sinh s}{\cosh s} = \frac{1 - e^{-2s}}{1 + e^{-2s}}.$$

A simple computation shows that

$$\sinh(2s) = 2 \sinh(s) \cosh(s) \tag{A.10}$$

and one easily checks that

$$0 \leq \tanh t \leq \min\{t, 1\}. \tag{A.11}$$

holds for $t \geq 0$.

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Declaration

I hereby affirm that the thesis at hand is independent work of myself and that work of others used herein is attributed as such. Furthermore, this thesis was neither submitted as whole, nor in part, to another board of examination in pursuit of attainment of an academic degree.

Würzburg, 17 February 2015

Marc Philipp Technau
born in Freiburg im Breisgau