Selfsimilarity of “Riemann’s Nondifferentiable Function”

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Abstract

This is an expository article about the series

$$f(x) = \sum_{n=1}^{\infty} \frac{1}{n^2} \sin(n^2 x),$$

which according to Weierstrass was presented by Riemann as an example of a continuous function without a derivative. An explanation is given of infinitely many selfsimilarities of the graph, from which the known results about the differentiability properties of $f(x)$ are obtained as a consequence.

Key words: Riemann’s nondifferentiable function, theta function, modular group, selfsimilarity, fractal.

AMS classification: primary: 26A27, secondary: 26A16, 10D12, 14K25.

1 Introduction

According to Weierstrass [22], in a talk to the Royal Academy of Sciences in Berlin on 18 July 1872, Riemann introduced the function

$$f(x) = \sum_{n=1}^{\infty} \frac{1}{n^2 \pi} \sin(n^2 \pi x) \tag{1.1}$$

in order to warn that continuous functions need not have a derivative. (The scaling with π will simplify later formulas.) Not succeeding in verifying that $f(x)$ is nowhere differentiable, Weierstrass proved this property instead for the series $\sum_{n \geq 0} a^{-n} \sin(b^n \pi x)$, with suitably chosen positive numbers a and b. This appeared first in print in Du Bois-Reymond [5]. According to Butzer and Stark [2], there are no other known sources which confirm Riemann’s role in the story.

Hardy [7, pp. 322-323] proved that “Riemann’s” function $f(x)$ is not differentiable in any irrational point x and also not differentiable in a large class of rational x. With a completely elementary but long proof, Gerver [6] succeeded in 1970 in showing that at every rational point $r = \frac{p}{q}$ with p and q both odd, $f(x)$ is differentiable, and has derivative equal to $-\frac{1}{2}$ at r. Furthermore he showed that at all other rational points the function is not differentiable. Other, shorter proofs were given by Smith [20], Queffelec [18], Mohr [16], Itatsu [11], Luther [15] and Holschneider and Tchamitchian [9]. For previous reviews on Riemann’s function, see Neuenschwander [17] and Segal [19]; the literature list of [2] contains many further references.

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Already for many years, a picture of the graph of $f(x)$, made by A.J. de Meijer, adorns the cover of the notes of the first semester analysis course in Utrecht. In it, the aforementioned differentiability properties at the rational points with not too large denominators can be distinguished quite clearly. However, another striking feature which immediately attracts the attention, is the repetition of similar patterns in decreasing sizes. See Figure 1.1 below. In local enlargements near the rational points these repeated patterns are even more impressive, cf. Figures 4.2 and 4.4. (The pictures, made by means of a dot matrix printer, just show the values of the functions for a large but finite number of values of x. As a result, points in the graph may be missing where the function is very steep.)

$-0.127 < x < 2.127$
$-0.845 < y < 0.845$

Figure 1.1: $y = \sum_{n=1}^{\infty} \frac{1}{n^2\pi} \sin(n^2\pi x)$

In the following discussion, it is convenient to work with the complex valued series

$$\phi(x) := \sum_{n=1}^{\infty} \frac{1}{in^2\pi} e^{n^2\pi i x}. \tag{1.2}$$

Note that $\phi(x) = f(x) - ig(x)$, where $g(x)$ is the corresponding cosine series, defined by

$$g(x) = \sum_{n=1}^{\infty} \frac{1}{n^2\pi} \cos(n^2\pi x). \tag{1.3}$$

See Figures 1.2, 1.3.

$-0.127 < x < 2.127$
$-0.845 < y < 0.845$

Figure 1.2: $y = \sum_{n=1}^{\infty} \frac{1}{n^2 \pi} \cos(n^2 \pi x)$

$-0.637 < x < 0.637$
$-0.477 < y < 0.477$

Figure 1.3: $x = g(t)$, $y = f(t)$

My starting point in attempting to understand the pictures was to apply the Poisson summation formula to $\phi(x)$. This was inspired by Smith [20], who used the Poisson summation formula, although he did not apply it to the function $\phi(x)$ itself. What I got was a formula which showed that $\phi(x)$ *is similar to* $\phi(\frac{-1}{x})$*, modulo a differentiable remainder term.*

Combined with the periodicity of $\phi(x)$ with period 2, the formula explains the observed selfsimilarities in the singularities of the graph of f. In fact, the eye is very sensitive to small hooks and pays much less attention to larger scale smooth perturbations. Figure 4.1 shows how much duller the remainder term is compared to the function $f(x)$ itself. As a free bonus, the differentiability properties of $f(x)$ at the rational points could be read off immediately from the formula.

It then dawned on me that this selfsimilarity formula was just an integrated version of the well-known transformation formula

$$\theta(x) = \theta(\frac{-1}{x}) \cdot e^{\frac{\pi i}{4}} \cdot x^{-\frac{1}{2}}, \ \ \text{Im } x > 0. \tag{1.4}$$

for the classical *theta function*

$$\theta(x) := \sum_{n \in \mathbf{Z}} e^{n^2 \pi i x}. \tag{1.5}$$

This series converges locally uniformly to a complex analytic function on the complex upper half plane

$$\mathcal{H} := \{x \in \mathbf{C} \mid \ \text{Im } x > 0\}. \tag{1.6}$$

Similarly, (1.2) defines a complex analytic function on $\mathcal{H}$, with derivative equal to

$$\phi'(x) = \tfrac{1}{2}(\theta(x) - 1), \ \ x \in \mathcal{H}. \tag{1.7}$$

Note that the theta function has no continuous limit at the real axis, the boundary of $\mathcal{H}$, in contrast with its primitive. The limit of the theta function is a distribution, which can be identified with $x \mapsto \text{Trace } (e^{-ix\Delta})$, where Δ denotes the Laplacian of the circle, cf. Duistermaat and Guillemin [4, pp. 45,46]. Unlike $\phi(x)$, this distribution is difficult to visualize.

The functional equation (1.4) had been found for $x = it$, $t > 0$ by Gauss (1808) and Cauchy (1817), whereas Poisson (1823) showed that it is a special case of a general summation formula. See Burkhardt [1, nr. 107, pp. 1339-1342]. According to Cauchy [3, p.157], Poisson also remarked that the formula holds for other complex x. Using the asymptotic expansion for $x = \frac{2}{q} + i\epsilon$, $\epsilon \downarrow 0$, Cauchy then used (1.4) in order to give a simple proof of the famous identity

$$\sum_{k=0}^{q-1} e^{2\pi i \frac{k^2}{q}} = c \cdot q^{\frac{1}{2}} \tag{1.8}$$

for *Gauss sums*. Here $c = 1$ if $q \in 4\mathbf{Z} + 1$ and $c = i$ if $q \in 4\mathbf{Z} - 1$. A formula with $\frac{2}{q}$ replaced by $\frac{p}{q}$ can be read off from (3.4).

The next idea is to combine the identity (1.4) with the periodicity $\theta(x + 2) = \theta(x)$. The mappings $\tau_2 : x \mapsto x + 2$ and $\sigma : x \mapsto \frac{-1}{x}$ generate a subgroup Γ_θ of the group Γ of fractional linear transformations

$$\gamma : x \mapsto \tfrac{ax+b}{cx+d}, \ \ a, b, c, d \in \mathbf{Z}, \ ad - bc = 1. \tag{1.9}$$

Γ and Γ_θ are called the *modular group* and the *theta modular group*, respectively. Combining (1.4) with the periodicity, we obtain for each $\gamma \in \Gamma_\theta$ a transformation formula of the form

$$\theta(x) = \theta(\gamma(x)) \cdot e^{\frac{\pi i}{4} m} \cdot q^{-\frac{1}{2}} (x - r)^{-\frac{1}{2}}. \tag{1.10}$$

Here $r = \frac{p}{q}$ is the rational number at which γ has a pole and m is an integer which only depends on r.

Integrating (1.10) from r to $x \in \mathcal{H}$ and then moving x to the real axis, (1.7) now leads to a selfsimilarity of $\phi(x)$ under the transformation γ, for every $\gamma \in \Gamma_\theta$. Again, the selfsimilarity is only modulo differentiable functions, see Theorem 4.2 for the detailed statement. The translation into corresponding similarities for $f(x)$ and $g(x)$ is straightforward. An expansion with arbitrarily many terms is given in Proposition 4.6.

At the same time, the selfsimilarity formula can be read as an asymptotic expansion of $\phi(x)$ as $x \to r$, from which it follows that $\phi(x)$ is not differentiable at r, and actually has a singularity of square root type at one side or at both sides of r. The pole points of the $\gamma \in \Gamma_\theta$ turn out to be the rational numbers $r = \frac{p}{q}$ for which not both p and q are odd. The singularities of the functions $f(x)$ and $g(x)$ at these points are classified in Table 4.4.

The rational numbers $s = \frac{p}{q}$ for which both p and q are odd can be obtained from the ones of the type even/odd by means of a translation over 1. With the notation $t_n(x) := e^{n^2\pi i x}/n^2\pi i$, we have

$$\phi(1+x) = \sum_{n \text{ even}} t_n(x) - \sum_{n \text{ odd}} t_n(x) = 2\sum_{n \text{ even}} t_n(x) - \sum_{n \in \mathbf{Z}} t_n(x) = \tfrac{1}{2}\phi(4x) - \phi(x). \quad (1.11)$$

In combination with the previous description of the singularity of $\phi(x)$ and $\phi(4x)$ at the points even/odd, this yields that $\phi(x)$ is differentiable at $x = s$, with derivative equal to $-\frac{1}{2}$. See Proposition 4.5.

Approximating an *irrational* real number ρ by means of continued fractions r, and using the uniformity of the asymptotics at the rational points r, we recover the result of Hardy [7, p. 323] that $f(x)$ and $g(x)$ are *not* of order $o(|x-\rho|^{\frac{3}{4}})$ as $x \to \rho$. See Proposition 5.2. This implies that $f(x)$ and $g(x)$ are not differentiable at any irrational point. In the other direction we verify that, at almost all irrational numbers, the Hölder exponent is arbitrarily close to $\frac{3}{4}$.

Our proofs are similar to the arguments which Hardy and Littlewood [8] used for their asymptotics of the real and imaginary part of the theta function $\theta(x)$, as $x \in \mathcal{H}$ approaches an irrational real number. See [8, p. 233]. Using the Poisson formula for harmonic functions, Hardy [7, Lemma 2.11] expressed the real and imaginary part of $\theta(x)$ in terms of $f(x)$ and $g(x)$, respectively. He then argues that $o(|x-\rho|^{\frac{3}{4}})$ behaviour of $f(x)$ or $g(x)$ would lead to conclusions about the asymptotics of $\theta(x)$ as $x \to \rho$ which are incompatible with the results of [8]. Our proof avoids the detour via the asymptotics of $\theta(x)$, at the cost of redoing some of the arguments concerning the approximation with continued fractions. I actually enjoyed this, although I am not an expert in number theory at all.

When writing this article, I wondered why the selfsimilarity formula was not used by everybody who studied $f(x)$: it was lying just around the corner, with the so well known automorphic (= selfsimilar) properties of the theta function. Then I saw in the article of Butzer and Stark [2] that Christoffel, in a letter to Prym dated 18 June, 1865, actually *did* have the formula. It is the one for $\gamma : x \mapsto \frac{-1}{x}$ which I got by applying the Poisson summation formula to $f(x)$. If only Christoffel would have recognized his "second transformation" as a selfsimilarity, he might have found the whole story. Via [2] I also found the article of Itatsu [11], in which the asymptotics at the rational points is obtained in the same way as here.

After having seen the selfsimilarity of $f(x)$, many readers will have reacted with: "Ah, a fractal." This concept has been popularized by Mandelbrot, who writes in the Introduction of [14]: "Fractal geometry is a new branch born belatedly from the crisis in mathematics that started when du Bois-Reymond 1875 first reported on a continuous nondifferentiable function constructed by Weierstrass." But no selfsimilarity is mentioned in the comments on $f(x)$ in [14, Section 39]. As for the role of the computer, of course in the old days computer pictures were not available to put one on the track. On the other hand, the mathematical analysis definitely is the more essential part of the story. Without it, one may look at the pictures with equal fascination, but with less understanding.

In the rest of the paper we give the results and proofs in much more detail. In order to make the presentation reasonably self-contained, we have included proofs of some of the well-known basic facts which we use. After reviewing the Poisson summation formula in Section 2, we present the selfsimilarity of the theta function in Section 3, together with a determination of the group $,_{\theta}$ and the exponents m. This leads in Section 4 to the selfsimilarity modulo differentiable functions of $\phi(x)$, together with the asymptotic description of $\phi(x)$ near the rational points. The irrational points are treated in Section 5; certainly there remain some interesting open questions here. We take a look at fixed points of $\gamma \in \, ,_{\theta}$ in Section 6.

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2 The Poisson Summation Formula

In the following proposition we will remain safely with our functions in the *Schwartz space* $\mathcal{S}(\mathbf{R})$ of the infinitely differentiable complex valued functions $\psi(x)$ on $\mathbf{R}$, such that, for all nonnegative integers a and b, the function $x \mapsto x^a \cdot \frac{d^b}{dx^b}\psi(x)$ is bounded on $\mathbf{R}$.

Proposition 2.1 *For each $\psi \in \mathcal{S}(\mathbf{R})$, let*

$$(\mathcal{F}\psi)(\nu) := \int_{-\infty}^{\infty} e^{-in\nu}\psi(n)\,dn$$

denote its Fourier transform. Then

$$\sum_{n\in\mathbf{Z}} \psi(n) = \sum_{m\in\mathbf{Z}} (\mathcal{F}\psi)(2\pi m).$$

Proof The function

$$\chi(x) := \sum_{n\in Z} \psi(x+n)$$

of x is smooth (C^∞) and periodic, with period equal to 1. Its Fourier expansion, evaluated at $x = 0$, therefore is equal to

$$\begin{aligned}
\sum_{n\in\mathbf{Z}} \psi(n) = \chi(0) &= \sum_{m\in\mathbf{Z}} \int_0^1 e^{-2\pi i m y}\chi(y)\,dy \\
&= \sum_{m\in\mathbf{Z}} \int_0^1 e^{-2\pi i m y} \sum_{n\in\mathbf{Z}} \psi(y+n)\,dy = \sum_{m\in\mathbf{Z}}\sum_{n\in\mathbf{Z}} \int_n^{n+1} e^{-2\pi i m(y-n)}\psi(y)\,dy \\
&= \sum_{m\in\mathbf{Z}}\sum_{n\in\mathbf{Z}} \int_n^{n+1} e^{-2\pi i m y}\psi(y)\,dy = \sum_{m\in\mathbf{Z}} \int_{-\infty}^{\infty} e^{-2\pi i m y}\psi(y)\,dy = \sum_{m\in\mathbf{Z}} (\mathcal{F}\psi)(2\pi m).
\end{aligned}$$

□

Alternatively the Poisson summation formula can be phrased as an identity

$$\sum_{n\in\mathbf{Z}} \delta_n = \mathcal{F}(\sum_{m\in\mathbf{Z}} \delta_{2\pi m})$$

between tempered distributions, elements of the dual space of $\mathcal{S}(\mathbf{R})$. Here $\delta_a = \delta_a(x) = \delta(x-a)$ denotes the Dirac delta function translated to a, or the unit mass at a.

The Poisson summation formula can be extended by continuity to Lebesgue integrable continuous functions ψ on $\mathbf{R}$ for which there exists a sequence $\psi_j \in \mathcal{S}(\mathbf{R})$ such that $\psi_j|_{\mathbf{Z}}$ and $(\mathcal{F}\psi_j)|_{2\pi\mathbf{Z}}$ converge to $\psi|_{\mathbf{Z}}$ and $(\mathcal{F}\psi)|_{2\pi\mathbf{Z}}$, respectively. The required convergence here is with respect to the sumnorm. It is this version which I first applied to "Riemann's function" (1.1), before using the explanation via the theta function.

3 The Selfsimilarity of the Theta Function

In the sequel we will use the convention that

$$x^a = |x|^a \, e^{ai \arg x} \;\text{ if }\; x \neq 0,\; a \in \mathbf{R}, \tag{3.1}$$

where we choose $0 \leq \arg x \leq \pi$ if $\mathrm{Im}\; x \geq 0$. With this convention, we have:

Lemma 3.1 *The theta function $\theta(x) := \sum_{n\in\mathbf{Z}} \exp(n^2\pi i x)$, defined for $x \in \mathcal{H}$, satisfies the functional relation*

$$\theta(x) = \theta(\frac{-1}{x}) \cdot e^{\frac{\pi i}{4}} \cdot x^{-\frac{1}{2}}$$

and the periodicity relation $\theta(x+2) = \theta(x)$.

Proof For each $x \in \mathcal{H}$, the term $\psi_x(n) := \exp(n^2\pi i x)$, when considered as a function of $n \in \mathbf{R}$, belongs to the Schwartz space $\mathcal{S}(\mathbf{R})$. The substitution of variables

$$n \mapsto e^{\frac{\pi i}{4}} \, (\pi x)^{-\frac{1}{2}} n \,+\, \frac{\nu}{2\pi x}$$

in the complex line integral

$$(\mathcal{F}\psi_x)(\nu) = \int_{-\infty}^{\infty} e^{-in\nu + n^2\pi i x}\, dn$$

yields that

$$(\mathcal{F}\psi_x)(\nu) = e^{\frac{\pi i}{4}} \, (\pi x)^{-\frac{1}{2}} \cdot \int_{-\infty}^{\infty} e^{-n^2}\, dn \cdot e^{-i\frac{\nu^2}{4\pi x}} = e^{\frac{\pi i}{4}} \, x^{-\frac{1}{2}} \cdot e^{-i\frac{\nu^2}{4\pi x}}.$$

Note that this substitution of variables involves a turn of the path of integration over an angle $\frac{\pi}{4} - \frac{\arg x}{2}$ in the complex plane. Substituting $\nu = 2\pi m$ and summing over $m \in \mathbf{Z}$, and applying Proposition 2.1 to $\psi = \psi_x$, we obtain (1.4). □

By induction we get a formula for the transformation of the theta function under each element of the theta modular group $,_\theta$. That is, for each $\gamma \in\, ,_\theta$ there exists an analytic function μ_γ on the upper half plane $\mathcal{H}$, such that

$$\theta(x) = \theta(\gamma(x)) \cdot \mu_\gamma(x),\;\; x \in \mathcal{H}, \gamma \in\, ,_\theta. \tag{3.2}$$

We will need an explicit description of $,_\theta$ and the *multiplier system* $\gamma \mapsto \mu_\gamma$, $\gamma \in\, ,_\theta$.

A fractional linear transformation, with arbitrary complex coefficients $a, b, c, d \in \mathbf{C}$ such that $ad - bc \neq 0$, can be viewed as the restriction to $\mathbf{C}$ of the action of the corresponding 2×2- matrix $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ on the complex projective plane $\mathbf{C} \cup \{\infty\}$, the space of 1-dimensional linear subspaces of $\mathbf{C}^2$. Here $x \in \mathbf{C}$ and ∞ correspond to the lines in $\mathbf{C}^2$ through $(x, 1)$ and $(1, 0)$, respectively.

Note that the mapping which assigns the fractional linear transformation γ to the matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}(2, \mathbf{Z})$ is a group homomorphism, with kernel equal to $\{\pm I\}$. Therefore it is no restriction to adopt the convention that $c > 0$ if $c \neq 0$ and $a = d = 1$ if $c = 0$.

If $c \neq 0$, then γ has a pole at

$$r = \tfrac{p}{q}, \text{ with } p := -d,\ q := c. \tag{3.3}$$

That is, $r = r_\gamma$ is the point x such that $\gamma(x) = \infty$, which makes it natural to define $r = \infty$ if $c = 0$. Note that the determinant condition $ad - bc = 1$ implies that p and q have no common factor, so the rational number $r = \frac{p}{q}$ is written in the usual reduced form. Also, $r_\gamma = r_{\gamma'}$ if and only if $\tau := \gamma' \circ \gamma^{-1}$ maps ∞ to itself. This means that the matrix of τ is upper triangular. Because it is integral and has determinant equal to 1, τ is a translation. Because the element $\sigma : x \mapsto \frac{-1}{x}$ of , $_\theta$ interchanges 0 and ∞, the set of pole points $\gamma^{-1}(\infty)$, $\gamma \in$, $_\theta$, is equal to the , $_\theta$-orbit of 0.

Lemma 3.2 *The , $_\theta$-orbit of* 0 *consists of* ∞*, together with the rational numbers* $r = \frac{p}{q}$ *with* p *even and* q *odd, or* p *odd and* q *even. The remaining rational numbers* $r = \frac{p}{q}$ *with* p *and* q *both odd constitute the , $_\theta$-orbit of* 1.

A fractional linear transformation belongs to , $_\theta$ if and only if it is defined by a matrix of the form $\begin{pmatrix} \text{odd} & \text{even} \\ \text{even} & \text{odd} \end{pmatrix}$ *or* $\begin{pmatrix} \text{even} & \text{odd} \\ \text{odd} & \text{even} \end{pmatrix}$. *The quotient space , /, $_\theta$ has three elements. , $_\theta$ is not a normal subgroup of , .*

Proof Write B for the set of rational numbers $\frac{p}{q}$ with p and q both odd, and $A := (\mathbf{Q} \cup \{\infty\}) \setminus B$. It is clear that τ_2 and σ leave B invariant, so B is invariant under , $_\theta$ and the same is true for its complement A. Furthermore, $1 \in B$ and $0 \in A$, hence , $_\theta \cdot 1 \subset B$ and , $_\theta \cdot 0 \subset A$. We have the desired equalities if we can prove that every rational number is in the , $_\theta$-orbit of 1 or 0.

For this purpose, we begin with the observation that by a translation $\tau_{2k} = (\tau_2)^k \in$, $_\theta$ over an even number $2k$, we can bring any rational number in the interval $]-1, 1]$. Now let $x = \frac{p}{q}$, with p and q integers without common factors, $q > 0$ and $-1 < x \leq 1$. If $x \neq 0$ and $x \neq 1$ then $0 < |p| < q$. There is an $l \in \mathbf{Z}$ such that $y := \tau_{2l} \circ \sigma(x) \in]-1, 1]$. Now y is in the , $_\theta$-orbit of x and the denominator of y, which is equal to $|p|$, is strictly smaller than the denominator q of x. Putting y in the role of x we can continue the process. This has to break off after at most q steps. To break off means that we have arrived at $y = 0$ or $y = 1$. It may be noted that this procedure is a continued fraction expansion with only even integers, which on the other hand are allowed to be negative. These do not have the convergence properties as the ones in Lemma 5.1.

For the description of , $_\theta$, write ˜, for the group of $\gamma \in$, with a matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, which modulo 2 is of the form $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ or $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Clearly , $_\theta \subset$ ˜, . If $\gamma \in$ ˜, has the matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, then $\gamma^{-1}(\infty) = \frac{-d}{c} \in A =$, $_\theta \cdot 0 =$, $_\theta \cdot \infty$, so there exists a $\delta \in$, $_\theta$ such that $\gamma^{-1}(\infty) = \delta^{-1}(\infty)$. Writing $\epsilon := \delta \circ \gamma^{-1}$, we have $\epsilon(\infty) = \infty$, or ϵ is a translation over an integer b, with matrix $\begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix}$. Because $\epsilon \in$ ˜, , b is even, which implies that $\epsilon \in$, $_\theta$. Because also $\delta \in$, $_\theta$, the conclusion is that $\gamma \in$, $_\theta$.

The homomorphism which reduces the matrix of $\gamma \in$, modulo 2 has as its kernel the group of γ's for which the matrix is odd on the diagonal and even on the antidiagonal, which is a subgroup of , $_\theta$. This reduction maps , onto the group G of invertible 2×2- matrices over $\mathbf{Z}/2\mathbf{Z}$, which has 6 elements, and , $_\theta$ onto the subgroup H consisting of $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. This proves that , /, $_\theta \simeq G/H$ has three elements. The last statement in the lemma results from the fact that H is not a normal subgroup of G. □

Lemma 3.3 *The multiplier μ_γ depends only on the pole point $r = r_\gamma$. If $r = \frac{p}{q}$, p and q integers without common factors and $q > 0$, then*

$$\mu_\gamma(x) = e^{\frac{\pi i}{4}m} \cdot q^{-\frac{1}{2}} \cdot (x-r)^{-\frac{1}{2}} = e^{\frac{\pi i}{4}} \cdot \frac{1}{q} \sum_{k=0}^{q-1} e^{\pi i \frac{p}{q} k^2} \cdot (x-r)^{-\frac{1}{2}}. \tag{3.4}$$

Here the integers

$$m = m(r) \in \mathbf{Z}/8\mathbf{Z}$$

in the exponent are determined recursively by

$$m(\infty) = 0,\ m(0) = 1, \tag{3.5}$$

$$m(r+2) = m(r), \tag{3.6}$$

$$m(\tfrac{-1}{r}) = m(r) - \operatorname{sign} r\,. \tag{3.7}$$

Proof If $\gamma, \delta \in$, $_\theta$, then $\theta(x) = \theta(\gamma(x)) \cdot \mu_\gamma(x) = \theta(\delta(\gamma(x)) \cdot \mu_\delta(\gamma(x)) \cdot \mu_\gamma(x)$, which leads to the composition rule $\mu_{\delta\circ\gamma}(x) = \mu_\delta(\gamma(x)) \cdot \mu_\gamma(x)$. This is similar to the chain rule $(\delta\circ\gamma)'(x) = \delta'(\gamma(x)) \cdot \gamma'(x)$ for the derivative. If γ has the coefficients a, b, c, d, then

$$\gamma'(x) = (cx+d)^{-2} = q^{-2}\,(x-r)^{-2} \ \text{ if } \ r = r_\gamma = \tfrac{p}{q},\ q > 0. \tag{3.8}$$

For $\gamma = \sigma : x \mapsto \frac{-1}{x}$, this is equal to $-\mu_\gamma(x)^4$. So we get by induction that $\mu_\gamma(x) = e^{\frac{\pi i}{4}m_\gamma} \cdot \gamma'(x)^{\frac{1}{4}}$, for a suitable function $\gamma \mapsto m_\gamma$: , $_\theta \to \mathbf{Z}/8\mathbf{Z}$. Here (3.8) suggests to use the convention that $-2\pi < \arg\gamma'(x) < 0$ for $x \in \mathcal{H}$, so that $\gamma'(x)^{\frac{1}{4}} = q^{-\frac{1}{2}}\,(x-r)^{-\frac{1}{2}}$ remains compatible with (3.1). We have proved the first identity in (3.4).

For the second identity in (3.4), we follow the proof of Cauchy [3, pp. 157-159] of (1.8). We start with the asymptotic expansion

$$\theta(r+i\epsilon) \approx \frac{1}{q\sqrt{\epsilon}} \sum_{k=0}^{q-1} e^{\pi i \frac{p}{q}k^2} \quad \text{as} \quad \epsilon \downarrow 0.$$

This can be derived by substituting $n = lq + k$ in (1.5) and viewing the sum over $l \in \mathbf{Z}$ as a Riemann sum for the integral of e^{-x^2}. On the other hand, because $\gamma(r+i\epsilon) \approx iC/\epsilon$ for a positive constant C, we get that $\theta(\gamma(r+i\epsilon))$ converges to 1, so $\gamma(r+i\epsilon)$ is asymptotically equal to the middle term in (3.4).

We now turn to the proof of (3.7). Because

$$\gamma'(x)^{\frac{1}{4}} = |\gamma'(x)|^{\frac{1}{4}} \cdot \exp(\tfrac{\pi i}{4}\,\tfrac{\arg\gamma'(x)}{\pi}),$$

the composition rule for the m_γ reads

$$m_{\delta\circ\gamma} = m_\delta + m_\gamma + \tfrac{1}{\pi}\,[\arg\,\delta'(\gamma'(x)) + \arg\,\gamma'(x) - \arg\,(\delta\circ\gamma)'(x)].$$

If we apply this to $\gamma = \sigma$, $r_\delta = \frac{p}{q}$ with $q > 0$, then the substitution of $x = i\epsilon$, $\epsilon \downarrow 0$ yields that

$$\delta'(\gamma(x)) = (q \cdot \tfrac{-1}{x} - p)^{-2} = (\tfrac{iq}{\epsilon} - p)^{-2}$$

has argument close to $-\pi$ and $\gamma'(x) = (i\epsilon)^{-2}$ has argument equal to $-\pi$. Finally the argument of

$$(\delta\circ\gamma)'(x) = \delta'(\gamma(x)) \cdot \gamma'(x) = (-q - i\epsilon p)^{-2} = (q + i\epsilon p)^{-2}$$

converges to 0 if $p > 0$ and to -2π if $p < 0$, keeping the point under the power sign in $\mathcal{H}$. Because $m_\sigma = 1$, it follows that $m_{\delta\circ\sigma} = m_\delta - \mathrm{sign}(r_\delta)$. The proof of the lemma is completed by noting that

$$r_{\delta\circ\sigma} = (\delta\circ\sigma)^{-1}(\infty) = \sigma^{-1}(r_\delta) = \tfrac{-1}{r_\delta}.$$

□

The recursion to which is alluded in the lemma, is the procedure which is described in the proof of Lemma 3.2, to get a pole point to 0 by a succession of translations over even numbers and reflections $x \mapsto \frac{-1}{x}$. This leads to a very effective algorithm for the computation of the $m(\frac{p}{q})$.

It follows from (3.7) that an increase of m by one corresponds to a passage $A_1 \to A_2 \to A_3 \to A_4 \to A_1$, where

$$\begin{aligned} A_1 &:= \{\tfrac{p}{q} \mid p \in 2\mathbf{Z},\ q \in 4\mathbf{Z}+1,\ q > 0\}, \\ A_2 &:= \{\tfrac{p}{q} \mid p \in 4\mathbf{Z}+1,\ q \in 2\mathbf{Z},\ q > 0\}, \\ A_3 &:= \{\tfrac{p}{q} \mid p \in 2\mathbf{Z},\ q \in 4\mathbf{Z}+3 = 4\mathbf{Z}-1,\ q > 0\}, \\ A_4 &:= \{\tfrac{p}{q} \mid p \in 4\mathbf{Z}+3,\ q \in 2\mathbf{Z},\ q > 0\}. \end{aligned}$$

That is,

$$m(\tfrac{p}{q}) \equiv k \bmod 4 \ \text{ if } \tfrac{p}{q} \in A_k. \tag{3.9}$$

This determines the multipliers up to a sign.

The signs however follow a quite subtle pattern, which can be described in terms of the *Jacobi symbols* $(\frac{n}{m}) = \pm 1$. These are defined for integers n and m such that m is positive and odd, $n \neq 0$ and $\gcd(n,m) = 1$, as follows.

$$(\tfrac{n}{m}) = \prod_{u=1}^{v} (\tfrac{n}{p_u}) \text{ if } m = \prod_{u=1}^{v} p_u,\ \ p_u > 2,\ p_u \text{ is prime.} \tag{3.10}$$

This includes the convention that $(\frac{n}{m}) = 1$ if $m = 1$. For p a prime > 2, n a nonzero integer, $(\frac{n}{p})$ is called a *Legendre symbol* and is defined by

$$(\tfrac{n}{p}) = 1 \text{ if } n \text{ is a square modulo } p,\ (\tfrac{n}{p}) = -1 \text{ otherwise.} \tag{3.11}$$

The Jacobi symbols have the following basic properties (3.12)-(3.16).

$$(\tfrac{n+m}{m}) = (\tfrac{n}{m}), \tag{3.12}$$
$$(\tfrac{n\cdot n'}{m}) = (\tfrac{n}{m})\cdot(\tfrac{n'}{m}), \tag{3.13}$$
$$(\tfrac{-1}{m}) = (-1)^{\frac{m-1}{2}}, \tag{3.14}$$
$$(\tfrac{2}{m}) = (-1)^{\frac{m^2-1}{8}}, \tag{3.15}$$
$$(\tfrac{n}{m})\cdot(\tfrac{m}{n}) = (-1)^{\frac{n-1}{2}\cdot\frac{m-1}{2}}. \tag{3.16}$$

All these equations hold as far as the Jacobi symbols were defined. For example, the *quadratic reciprocity law* (3.16) holds if n and m both are positive odd integers without common factors. See [13, Part I, Chap. 6].

So, in contrast with our $m(\frac{p}{q})$'s, the Jacobi symbols are defined in terms of the prime factor decompositions of p and q, and for the prime factors in terms of quadratic residues. I found the following description of the multipliers in Knopp [12, p. 51].

Theorem 3.4 *If $\gamma \in \Gamma_\theta$ has its pole at $r = \frac{p}{q}$ with $q > 0$, $\gcd(p,q) = 1$, then*

$$\theta(x) = \theta(\gamma(x)) \cdot e^{\frac{\pi i}{4}q} \cdot (\tfrac{-p}{q}) \cdot q^{-\frac{1}{2}}\,(x-r)^{-\frac{1}{2}} \quad \textit{if } q \textit{ is odd},$$
$$\theta(x) = \theta(\gamma(x)) \cdot e^{\frac{\pi i}{4}(p+1)} \cdot (\tfrac{q}{|p|}) \cdot q^{-\frac{1}{2}}\,(x-r)^{-\frac{1}{2}} \quad \textit{if } p \textit{ is odd}.$$

Proof Let us temporarily write $\zeta := e^{\frac{\pi i}{4}}$. From (3.7) and the remark after Lemma 3.3, it follows that

$$\epsilon(\tfrac{p}{q}) := \zeta^{m(\frac{p}{q})-q} = \zeta^{m(\frac{-q\cdot s}{|p|})+s-q} = \pm 1, \quad s := \text{sign } p, \tag{3.17}$$

if q is positive odd and p is even. The equations (3.6) for odd q are equivalent to

$$\epsilon(\tfrac{p+2q}{q}) = \epsilon(\tfrac{p}{q}) \ \text{ if } q \text{ is odd}, \ q > 0. \tag{3.18}$$

The other cases of (3.6) are equivalent to

$$\text{If} q+2p > 0, \text{ then: } \epsilon(\tfrac{p}{q}) = \epsilon(\tfrac{p}{q+2p}) \Longleftrightarrow p/2 \text{ is even}. \tag{3.19}$$
$$\text{If} q+2p < 0, \text{ then: } \epsilon(\tfrac{p}{q}) = \epsilon(\tfrac{-p}{-q-2p}) \Longleftrightarrow (p-q+1)/2 \text{ is even}. \tag{3.20}$$

By repeated translations of $\frac{p}{q}$ and $\frac{-q}{p}$ over even numbers, we arrive at $q = 1$, for which $\epsilon(p) = 1$. The relation with the Jacobi symbols follows from the fact that if we replace $\epsilon(\frac{p}{q})$ by $(\frac{-p}{q})$, then we get the same properties (3.18)-(3.20), and $(\frac{-p}{q}) = 1$ if $q = 1$. The conclusion therefore is that $\epsilon(\frac{p}{q}) = (\frac{-p}{q})$ if p is even and $q > 0$ is odd.

Indeed, the property (3.18) for the Jacobi symbols follows from (3.12). For the proof of the properties (3.19), (3.20) for the Jacobi symbols, we write, for m positive odd and $n \neq 0$:

$$n = 2^k \nu\, s, \ \ \nu \text{ positive and odd}, \ s = \text{sign } n.$$

Using (3.13), (3.15), (3.14) and (3.16), this yields

$$(\tfrac{n}{m}) = (-1)^{\frac{m^2-1}{8}k + \frac{m-1}{2}\frac{1-s}{2} + \frac{\nu-1}{2}\frac{m-1}{2}} \cdot (\tfrac{m}{\nu}).$$

Using the same equation with m replaced by $m+2n$, and the fact that (3.18) implies that $(\frac{m}{\nu}) = (\frac{m+2n}{\nu})$, the properties (3.19), (3.20), with $\epsilon(\frac{p}{q})$ replaced by $(\frac{-p}{q})$, can be deduced. $\square$

Using (3.15) once more, the results can also be summarized as follows:

Table 3.5 *If $p, q \in \mathbf{Z}$, $q > 0$, $\gcd(p,q) = 1$, not both p and q odd, then $m = m(\frac{p}{q}) \in \mathbf{Z}/8\mathbf{Z}$ is given by:*

$$\text{If } q \in 4\mathbf{Z}+1 \text{ then: } m \equiv 1 \text{ if } (\tfrac{p/2}{q}) = 1, \;\; m \equiv 5 \text{ if } (\tfrac{p/2}{q}) = -1.$$
$$\text{If } q \in 4\mathbf{Z}+3 \text{ then: } m \equiv 3 \text{ if } (\tfrac{p/2}{q}) = 1, \;\; m \equiv 7 \text{ if } (\tfrac{p/2}{q}) = -1.$$
$$\text{If } p \in 4\mathbf{Z}+1 \text{ then: } m \equiv 2 \text{ if } (\tfrac{q/2}{|p|}) = 1, \;\; m \equiv 6 \text{ if } (\tfrac{q/2}{|p|}) = -1.$$
$$\text{If } p \in 4\mathbf{Z}+3 \text{ then: } m \equiv 0 \text{ if } (\tfrac{q/2}{|p|}) = 1, \;\; m \equiv 4 \text{ if } (\tfrac{q/2}{|p|}) = -1.$$

4 The Primitive of Theta

We now turn to the study of the function

$$\phi(x) := \sum_{n=1}^{\infty} \frac{1}{in^2\pi} e^{n^2\pi i x},$$

introduced before in (1.2). Because of the uniform convergence of the series, this defines a continuous function of $x \in \mathbf{R}$. Actually one has the following uniform Hölder estimate, which even holds on the closure of the upper half plane.

Lemma 4.1 *There exists a constant C such that*

$$|\phi(x) - \phi(y)| \leq C|x-y|^{\frac{1}{2}}$$

holds for all $x, y \in \mathbf{R}$.

Proof Write $\phi(x) = A_N(x) + B_N(x)$, with

$$A_N(x) := \sum_{n=1}^{N} \frac{1}{in^2\pi} e^{n^2\pi i x}, \quad B_N(x) := \sum_{n=N+1}^{\infty} \frac{1}{in^2\pi} e^{n^2\pi i x}.$$

Then $\frac{d}{dx}\frac{1}{in^2\pi} e^{n^2\pi i x} = e^{n^2\pi i x}$ has absolute value ≤ 1, so $|A_N(x) - A_N(y)| \leq N|x-y|$. On the other hand,

$$|B_N(x)| \leq \sum_{n=N+1}^{\infty} \frac{1}{n^2\pi} \leq \frac{1}{N\pi}.$$

Combining these estimates, we get

$$|\phi(x) - \phi(y)| \leq N|x-y| + \frac{2}{N\pi}.$$

The minimum of the right hand side as a function of $N \in \mathbf{R}$ is attained for $N = (\frac{2}{|x-y|\pi})^{\frac{1}{2}}$, and is equal to $2\,(\frac{2}{\pi}|x-y|)^{\frac{1}{2}}$. Replacing the optimal $N \in \mathbf{R}$ by a positive integer at a bounded distance, we get the desired estimate. $\square$

We now turn to selfsimilarity of $\phi(x)$ modulo differentiable functions which was announced in the introduction.

Theorem 4.2 *Let $\gamma \in \Gamma_\theta$ have its pole at $r = \frac{p}{q}$, with $p, q \in \mathbf{Z}$, $q > 0$, $\gcd(p,q) = 1$. Write $m = m(r)$. Then the function $\phi(x)$ satisfies*

$$\phi(x) = \phi(r) + e^{\frac{\pi i}{4}m} \cdot q^{-\frac{1}{2}} \cdot (x-r)^{\frac{1}{2}} - \tfrac{1}{2}(x-r) + e^{\frac{\pi i}{4}m} \cdot q^{\frac{3}{2}} \cdot (x-r)^{\frac{3}{2}} \cdot \phi(\gamma(x)) + \psi(x) \quad (4.1)$$

for $x \in \mathbf{R}$. Here the function $\psi(x) = \psi_r(x)$ depends only on the pole point r. It is differentiable, $\psi(r) = 0$ and the derivative is given by

$$\psi'(x) = -\tfrac{3}{2} e^{\frac{\pi i}{4}m} \cdot q^{\frac{3}{2}} \cdot (x-r)^{\frac{1}{2}} \cdot \phi(\gamma(x)).$$

Proof The fact that in (1.2) the sum is over the positive integers, whereas in the definition (1.5) the convention is to sum over all integers, makes that $\theta(x)$ is not quite equal to the derivative of $\phi(x)$, but satisfies the equation (1.7) instead. Substituting (3.2), we get

$$\phi'(x) = \tfrac{1}{2}\left(\theta(x) - 1\right) = \tfrac{1}{2}\theta(\gamma(x)) \cdot \mu_\gamma(x) - \tfrac{1}{2} = \phi'(\gamma(x)) \cdot \mu_\gamma(x) + \tfrac{1}{2}\mu_\gamma(x) - \tfrac{1}{2}.$$

Integrating this from ξ to x in the upper half plane $\mathcal{H}$ and performing a partial integration, we can rewrite this as

$$\begin{aligned} \phi(y)\Big/_{y=\xi}^{y=x} &= \phi(\gamma(y)) \cdot \tfrac{\mu_\gamma(y)}{\gamma'(y)} \Big/_{y=\xi}^{y=x} - \textstyle\int_\xi^x \phi(\gamma(y)) \cdot \frac{d}{dy} \frac{\mu_\gamma(y)}{\gamma'(y)}\, dy \\ &\quad + \tfrac{1}{2} \textstyle\int_\xi^x \mu_\gamma(y)\, dy - \tfrac{1}{2}(x-\xi). \end{aligned} \quad (4.2)$$

Substitution of (3.4) and (3.8) yields that

$$\frac{\mu_\gamma(x)}{\gamma'(x)} = e^{\frac{\pi i}{4}m} \cdot q^{\frac{3}{2}} \cdot (x-r)^{\frac{3}{2}}$$

and the primitive of μ_γ is a multiple of $(x-r)^{\frac{1}{2}}$. This implies that (4.2) has a continuous limit if we let the variables ξ, y, x become real. With the choice of $\xi = r$, (4.2) then becomes (4.1), with

$$\psi(x) = -\tfrac{3}{2} e^{\frac{\pi i}{4}m} \cdot q^{\frac{3}{2}} \cdot \int_r^x (y-r)^{\frac{1}{2}} \cdot \phi(\gamma(y))\, dy. \quad (4.3)$$

That $\psi(x)$ only depends on r follows from the fact that if $\gamma, \tilde{\gamma} \in \Gamma_\theta$ have the same pole point, then $\tilde{\gamma} = \tau \circ \gamma$ for a translation τ over an even integer. Hence $\phi \circ \tilde{\gamma} = \phi \circ \tau \circ \gamma = \phi \circ \gamma$. □

For each nonnegative integer k and real number α with $0 < \alpha < 1$, we write $C^{k,\alpha}(\mathbf{R})$ for the space of functions on $\mathbf{R}$ which are k times differentiable and for which the k-th order derivative h satifies locally uniform Hölder estimates

$$|h(x) - h(y)| \leq C|x-y|^\alpha$$

with Hölder exponent α. Then $\phi \in C^{0,\frac{1}{2}}(\mathbf{R})$ and $\psi_r \in C^{1,\frac{1}{2}}(\mathbf{R})$.

From (4.1) we immediately read off the asymptotic behaviour of $\phi(x)$ at the points r_γ, $\gamma \in \Gamma_\theta$:

Lemma 4.3 *If, in the notation of Theorem 4.2, we write*

$$\sigma_r(x) := \phi(r) + e^{\frac{\pi i}{4}m} \cdot q^{-\frac{1}{2}} \cdot (x-r)^{\frac{1}{2}} - \tfrac{1}{2}(x-r) \tag{4.4}$$

for the leading terms of the asymptotic expansion of $\phi(x)$ *at* $x = r = r_\gamma$*, then*

$$|\phi(x) - \sigma_r(x)| \leq \tfrac{\pi}{3}\, q^{\frac{3}{2}} \cdot |x-r|^{\frac{3}{2}}.$$

Proof Use that

$$\pi\, |\phi(x)| \leq \sum_{n=1}^{\infty} \tfrac{1}{n^2} = \tfrac{\pi^2}{6}. \tag{4.5}$$

The identity on the right is well-known. A proof can be given by observing that the left and right hand side of

$$\sum_{n \in \mathbf{Z}} \tfrac{1}{(z-n)^2} = \left(\tfrac{\pi}{\sin(\pi z)}\right)^2 = \tfrac{2\pi^2}{1-\cos 2\pi z} \tag{4.6}$$

are meromorphic functions of z, with the same poles and asymptotic behaviour as $z \to \infty$. So the difference is entire and vanishes at ∞, and therefore vanishes identically in view of Liouville's theorem. The constant term of the left hand side of (4.6) is equal to $2\sum_{n\geq 1} n^{-2}$ and that of the right hand side is equal to $\pi^2/3$. □

Recall from Lemma 3.2 that the $r = r_\gamma$, $\gamma \in\ ,_\theta$, are precisely the rational numbers $\frac{p}{q}$ such that $p, q \in \mathbf{Z}$, $q > 0$, $\gcd(p,q) = 1$ and not both p and q odd. The conclusion is that $\phi(x)$ has singularities of square root nature at each of these rational points, which lie dense on the real axis. The "strength factor" $q^{-\frac{1}{2}}$ in front of $(x-r)^{\frac{1}{2}}$ in (4.4) makes that the singularity is the most pronounced for the "simple"rational numbers, the ones with a small denominator.

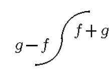
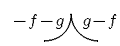
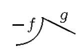
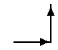
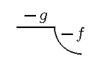
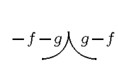
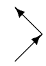
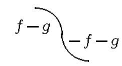
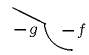
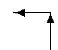
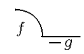
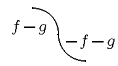
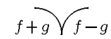
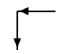
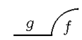
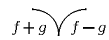
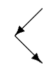
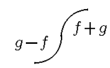
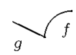
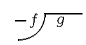
For the singularities of $f(x)$ and $g(x)$ we have to take the real and imaginary part of 4.4. Also note that, according to the convention in (3.1):

$$(x-r)^{\frac{1}{2}} = i \cdot |x-r|^{\frac{1}{2}} \text{ if } x < r.$$

If p is even and q is odd, then $m = m(r)$ is odd and we find square root type behaviour for $f(x)$ at both sides of r, with a factor $\pm(2q)^{-\frac{1}{2}}$ in front. On the other hand, if p is odd and q is even, then m is even and the real part of either $e^{\frac{\pi i}{4}m}$ or its multiple by i is equal to zero. It follows that at one side of r, $f(x)$ has a derivative equal to $-\frac{1}{2}$. At the other side of r, $f(x)$ has square root type behaviour, with a factor $\pm q^{-\frac{1}{2}}$ in front. For $g(x)$ we get the same conclusions, but with derivative $-\frac{1}{2}$ replaced by derivative equal to 0. The conclusions show that the Hölder exponent $\frac{1}{2}$ for $f(x)$ and $g(x)$ cannot be improved.

Using Table 3.5, we can summarize the eight possible cases in Table 4.4 below. In the diagrams, square root type behaviour is represented by a vertical curved arc, up or down according to the sign in front of the square root. A finite derivative at one side is represented by a straight line segment with the corresponding slope. The oriented curve $x \to \phi(x)$ in the complex plane has no well-defined velocity, but it approaches $\phi(x)$ infinitely fast from a well-defined direction as $x \to r$. The diagram for $\phi(x)$ depicts these directions. For a proper understanding of the relations between the diagrams, note that $\phi(x) = f(x) - ig(x)$.

Table 4.4 *The types of singularities which occur are:*

m mod 8	$r = \frac{p}{q}$	Ex.	$f(x)$	$\phi(x)$	$g(x)$
1	$p \in 2\mathbf{Z},\ q \in 4\mathbf{Z}+1,\ (\frac{p/2}{q}) = 1$	0			
2	$q \in 2\mathbf{Z},\ p \in 4\mathbf{Z}+1,\ (\frac{q/2}{\lvert p \rvert}) = 1$	$\frac{1}{2}$			
3	$p \in 2\mathbf{Z},\ q \in 4\mathbf{Z}+3,\ (\frac{p/2}{q}) = 1$	$\frac{2}{3}$			
4	$q \in 2\mathbf{Z},\ p \in 4\mathbf{Z}+3,\ (\frac{q/2}{\lvert p \rvert}) = -1$	$\frac{3}{4}$			
5	$p \in 2\mathbf{Z},\ q \in 4\mathbf{Z}+1,\ (\frac{p/2}{q}) = -1$	$\frac{4}{5}$			
6	$q \in 2\mathbf{Z},\ p \in 4\mathbf{Z}+1,\ (\frac{q/2}{\lvert p \rvert}) = -1$	$-\frac{3}{4}$			
7	$p \in 2\mathbf{Z},\ q \in 4\mathbf{Z}+3,\ (\frac{p/2}{q}) = -1$	$-\frac{2}{3}$			
0	$q \in 2\mathbf{Z},\ p \in 4\mathbf{Z}+3,\ (\frac{q/2}{\lvert p \rvert}) = 1$	$-\frac{1}{2}$			

We now take a look at the remainder term $\psi_r(x)$ in the equation (4.1).

$-0.127 < x < 2.127$
$-0.845 < y < 0.845$

Figure 4.1: $y = \text{Re } \psi_0(x)$

Using (4.4), we can rewrite (4.1) in the form

$$\phi(x) = \sigma_r(x) + \phi(\gamma(x)) \cdot e^{\frac{\pi i}{4} m} \cdot q^{\frac{3}{2}} \cdot (x - r)^{\frac{3}{2}} + \psi_r(x),$$

where $\psi_r(x) \in C^{1,\frac{1}{2}}((\mathbf{R})$. It follows from Proposition 4.6 below, with $l = 2$, that

$$\psi_r(x) = \mathrm{O}(|x - r|^{\frac{5}{2}}) \text{ as } x \to r.$$

So in addition to being smoother, the remainder term is also asymptotically of smaller order as $x \to r$. Figure 4.1 depicts the real part of $\psi_r(x)$ for $r = 0$, $\gamma : x \mapsto \frac{-1}{x}$.

The selfsimilarity modulo differentiable functions under the action of the fractional linear transformations $\gamma \in {}_{\theta}$ is quite spectacular: if x converges to $r = r_\gamma$, then $\gamma(x)$ converges to infinity. Due to the periodicity of ϕ, there is an infinite repetition of the same pattern of singularities, and γ transforms this to a sequence of repeated patterns which converges to r, at a distances from r of the form a constant times $\frac{1}{n}$ for the n-th pattern. The slow convergence of $\frac{1}{n}$ towards 0 as $n \to \infty$ makes that in the pictures very many repetitions of the patterns are visible.

Because $\phi(\gamma(x))$ is multiplied with a constant times $|x - r|^{\frac{3}{2}}$, the pattern is of the same order of magnitude as the estimate in Lemma 4.3 for the remainder term. In this sense Lemma 4.3 is optimal.

For $f(x)$ and $g(x)$ we get that near r we have to add a pattern which is proportional to $|x - r|^{\frac{3}{2}}$ times $\pm f$, $\pm g$, or $\pm f \pm g$, depending on the value of m and on the side of r. We have indicated this in Table 4.4 by writing the corresponding letters at the various branches of the diagrams.

Figure 4.2 is an enlargement near $x = \frac{1}{2}$ of the graph of $f(x)$. On the right of $x = \frac{1}{2}$ we see an infinite repetition of the graph of the function $g(x)$, see Figure 1.2

$0.498 < x < 0.563$

$0.349 < y < 0.398$

Figure 4.2: $y = f(x)$ near $x = \frac{1}{2}$

In order to facilitate the recognition of the patterns at the points with square root behaviour at both sides, we also provided a picture of the graph of $f(x) + g(x)$ in Figure 4.3. This one occurs to the right of $x = 0$.

$-0.127 < x < 2.127$
$-0.845 < y < 0.845$

Figure 4.3: $y = f(x) + g(x)$

Note that $-f(x) + g(x)$ is obtained by the reflection $x \mapsto -x$. For the behaviour at the other rational points we have:

Proposition 4.5 *The behaviour of $\phi(x)$ for x near 1 can be read off from*

$$\phi(1+x) = \tfrac{\pi i}{12} - \tfrac{1}{2}x + e^{\frac{\pi i}{4}} \cdot x^{\frac{3}{2}} \cdot [4\phi(\tfrac{-1}{4x}) - \phi(\tfrac{-1}{x})] + \chi(x), \tag{4.7}$$

where $\chi(x) \in C^{1,\frac{1}{2}}(\mathbf{R})$ is given by $\chi(0) = 0$ and

$$\chi'(x) = -\tfrac{3}{2}\, e^{\frac{\pi i}{4}} \cdot x^{\frac{1}{2}} \cdot [2\phi(\tfrac{-1}{4x}) - \phi(\tfrac{-1}{x})].$$

At each point $s = \frac{p}{q}$ with p and q both odd, $q > 0$, $\gcd(p,q) = 1$, we have

$$|\phi(y) - [\phi(s) - \tfrac{1}{2}(y-s)]| \leq \tfrac{5\pi}{3}\, q^{\frac{3}{2}} \cdot |y-s|^{\frac{3}{2}} \quad \textit{for all} \;\; y \in \mathbf{R}. \tag{4.8}$$

In particular, $\phi(y)$ is differentiable at $y = s$, with derivative equal to $-\frac{1}{2}$.

Proof The assumptions for s imply that $r := s - 1 = \frac{p-q}{q} = \frac{u}{q}$, with $u = p - q$ even, $q > 0$ odd and $\gcd(u,q) = 1$. Also, $4r = \frac{v}{q}$, with $v = 4u$ even and $\gcd(v,q) = 1$. Finally, using Theorem 3.4 and (3.13), (3.15), we see that $m := m(r) = m(4r)$.

Let us write $\phi(x) = \sigma_r(x) + R_r(x)$, with $\sigma_r(x)$ as in (4.4). Then $\frac{1}{2}\sigma_{4r}(4x) - \sigma_r(x) = \frac{1}{2}\phi(4r) - \phi(r) - \frac{1}{2}(x - r)$, where the essential feature is the cancellation of the square root terms. Now (1.11) yields

$$\phi(x+1) = \tfrac{1}{2}\,\phi(4x) - \phi(x) = \tfrac{1}{2}\,\phi(4r) - \phi(r) - \tfrac{1}{2}\,(x-r) + \tfrac{1}{2}R_{4r}(4x) - R_r(x).$$

For $r = 0$, we have $r = 4r = r_\gamma$, with $\gamma : x \to \frac{-1}{x}$. Reading R_r and R_{4r} off from (4.1), we get (4.7). On the other hand, writing $x + 1 = y$, $y - s = x - r$, the estimate in Lemma 4.3 leads to

$$|\tfrac{1}{2}R_{4r}(4x) - R_r(x)| \leq \tfrac{\pi}{3} \cdot q^{\frac{3}{2}} \cdot (\tfrac{1}{2}|4x - 4r|^{\frac{3}{2}} + |x - r|^{\frac{3}{2}}| \leq \tfrac{5\pi}{3}\, q^{\frac{3}{2}}\, |y-s|^{\frac{3}{2}}.$$

□

$0.96 < x < 1.04$
$-0.03 < y < 0.03$

Figure 4.4: $f(x)$ near $x = 1$

$-0.127 < x < 2.127$
$-0.845 < y < 0.845$

Figure 4.5: $y = \frac{3}{8}[4f(x) + 4g(x) - f(4x) - g(4x)]$

At the rational points $s = \frac{p}{q}$ with p and q both odd, the functions $f(x)$ and $g(x)$ are differentiable, but superimposed on the linear approximation we find an infinitely repeating pattern of singularities converging to s, of order of magnitude $|x-s|^{\frac{3}{2}}$. At $s = 1$ the singularity pattern has the shape of $k(\frac{-1}{4x})$, where $k(x) := 4f(x) + 4g(x) - f(4x) - g(4x)$. See Figures 4.4 and 4.5. As for the remainder term $\psi(x)$, we have that $\chi(x) = \mathrm{O}(|x|^{\frac{5}{2}})$ as $x \to 0$.

We conclude this section with the observation that the partial integration, which was used in the proof of Theorem 4.2, can be iterated. This results in an expansion of $\phi(x)$ in terms of functions of class $C^{k,\frac{1}{2}}(\mathbf{R})$, $k = 1, 2, \ldots$.

For this, we will make use of the functions $\phi_k(x)$ defined by

$$\phi_k(x) = \sum_{n=1}^{\infty} \tfrac{1}{(n^2 \pi i)^k} \, e^{n^2 \pi i x}, \tag{4.9}$$

for positive integral k. These are complex analytic functions on the upper half plane, and

$$\frac{d\phi_k}{dx}(x) = \phi_{k-1}(x), \; \frac{d^{k-1}\phi_k}{dx^{k-1}}(x) = \phi_1(x) = \phi(x). \tag{4.10}$$

It follows that $\phi_k(x)$ has a continuous extension on the closure of the complex upper half plane, to a function of class $C^{k,\frac{1}{2}}$. Finally,

$$\sup_x |\phi_k(x)| = |\phi_k(0)| = \pi^{-k} \sum_{n=1}^{\infty} n^{-2k} = \pi^{-k} \, \zeta(2k), \tag{4.11}$$

where $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$ is Riemann's zeta function.

As a side remark, Hardy [7] and later authors investigated the differentiability properties of $\phi_k(x)$ also for nonintegral real values of k, $k > \frac{1}{2}$. One could also use the interpretation

$$\phi_k(x) = (\frac{d}{dx})^{1-k} \, \phi(x),$$

where the "fractional integration" $(\frac{d}{dx})^{1-k}$ is a pseudodifferential operator of order $1-k$. This is a singular integral operator, of which the action on singularities is of a local nature. Also, it has good continuity properties with respect to Hölder norms. See Taylor [21, Ch. II, §2 and Ch. XI, Thm. 2.5].

Proposition 4.6 *For every $\gamma \in \,,_{\theta}$ and every nonnegative integer l, we have, with the notation of Theorem 4.2:*

$$\begin{aligned} \phi(x) = \quad & \phi(r) + e^{\frac{\pi i}{4} m} \, q^{-\frac{1}{2}} \, (x-r)^{\frac{1}{2}} - \tfrac{1}{2}(x-r) \\ & + e^{\frac{\pi i}{4} m} \cdot \{ \sum_{k=1}^{l} a_k \, (x-r)^{k+\frac{1}{2}} \cdot \phi_k(\gamma(x)) + b_l \int_r^x (y-r)^{l-\frac{1}{2}} \cdot \phi_l(\gamma(y)) \, dy \}, \end{aligned}$$

where the constants are given by

$$\begin{aligned} a_k &:= q^{2k-\frac{1}{2}} \, (-1)^{k-1} \prod_{j=1}^{k-1} (j + \tfrac{1}{2}), \\ b_l &:= -a_l \cdot (l + \tfrac{1}{2}) = a_{l+1}/q^2. \end{aligned}$$

Proof For $l = 1$, this is just (4.1). The result now follows by induction on l, for which we observe that (3.8) and a partial integration implies that

$$\begin{aligned} & \int_r^x (y-r)^{l-\frac{1}{2}} \cdot \phi_l(\gamma(y))\, dy \\ = & \int_r^x (y-r)^{l-\frac{1}{2}} \cdot \frac{d\phi_{l+1}}{dy}(\gamma(y))\, dy = \int_r^x q^2\,(y-r)^{l+2-\frac{1}{2}} \cdot \frac{d}{dy}\phi_{l+1}(\gamma(y))\, dy \\ = & \; q^2\,(y-r)^{l+1+\frac{1}{2}} \cdot \phi_{l+1}(\gamma(y)) - \int_r^x q^2\,(l+1+\tfrac{1}{2})\,(y-r)^{l+1-\frac{1}{2}} \cdot \phi_{l+1}(\gamma(y))\, dy. \end{aligned}$$

□

5 The Irrational Points

Let ρ be an irrational real number. The idea which first comes to mind in order to prove that $f(x)$ is not differentiable at ρ is to approximate ρ with rational numbers r which are not quotients of odd integers, and use the square root type of singularities of $f(x)$ at r in order to conlude sufficiently wild behaviour of $f(x)$ at ρ.

This program can be carried out, but in a somewhat subtle way. In the following explanation, "constant" means independent of $r = r_\gamma = \frac{p}{q}$ and ρ. The square root term in (4.1) is equal to a constant times $q^{-\frac{1}{2}}(x-r)^{\frac{1}{2}}$, whereas the remainder term can be estimated by a constant times $q^{\frac{3}{2}}(x-r)^{\frac{3}{2}}$, which is equal to the previous one times $q^2(x-r)$. Because we want to use this with $|x-r|$ of the same order of magnitude as $|\rho - r|$, we need that $r = \frac{p}{q}$ is an approximation of ρ of an order at most $\frac{1}{q^2}$. This, and a little bit more, is taken care of by the following

Lemma 5.1 *Let $\rho \in \mathbf{R}$ be irrational and let $r_n = \frac{p_n}{q_n}$ be the sequence of continued fraction approximations of ρ. Here $p_n, q_n \in \mathbf{Z}$, $q_n > 0$, $\gcd(p_n, q_n) = 1$. Then we have, for every n:*

$$|\frac{p_n}{q_n} - \rho| < \frac{1}{{q_n}^2} \tag{5.1}$$

and

$$p_{n-1},\ q_{n-1},\ p_n,\ q_n \ \text{ are not all odd.} \tag{5.2}$$

It follows that a subsequence of the continued fraction approximations belongs to the Γ_θ-orbit of ∞, that is, are not of the form odd/odd. Finally, the even numbered r_n increase monotonously towards ρ and the odd numbered r_n decrease monotonously towards ρ.

Proof For an introduction to continued fractions, see Hardy and Wright [10, Ch. X]. For the convenience of the reader, we repeat here what we need.

In order to obtain the continued fraction of ρ, one starts with the integer $a_0 \in]\rho - 1, \rho[$, or $\xi_0 := \rho - a_0 \in]0,1[$. Then, by induction on $n \geq 1$, one finds positive integers a_n such that

$$\xi_n = \tfrac{1}{\xi_{n-1}} - a_n \in]0,1[.$$

Reading these equations backward, we get

$$\rho = a_0 + \xi_0,\ \tfrac{1}{\xi_0} = a_1 + \xi_1, \ldots,\ \tfrac{1}{\xi_{n-1}} = a_n + \xi_n.$$

For any sequence of real numbers α_n, with $\alpha_n > 0$ for $n \geq 1$, one defines the *continued fraction with partial quotients* $\alpha_0, \alpha_1, \ldots, \alpha_n$ as:

$$\rho_n := [\alpha_0, \alpha_1, \ldots, \alpha_n] := \alpha_0 + 1/\alpha_1 + 1/ \ldots + 1/\alpha_n.$$

With this notation, we have

$$\rho = [a_0, a_1, \ldots, a_{n-1}, a_n + \xi_n]. \tag{5.3}$$

Now *the continued fraction approximations* r_n *of* ρ are defined by replacing the remainder ξ_n by 0:

$$r_n := [a_0, a_1, \ldots, a_{n-1}, a_n]. \tag{5.4}$$

It follows by induction on n that

$$\rho_{n+1} = \frac{\alpha_{n+1}\,\delta_n + \delta_{n-1}}{\alpha_{n+1}\,\epsilon_n + \epsilon_{n-1}} \quad \text{if} \quad \rho_n = \frac{\delta_n}{\epsilon_n}.$$

For the induction step one observes that

$$\begin{aligned}\rho_{n+1} = [\alpha_0, \alpha_1, \ldots, \alpha_{n-1}, \alpha_n + 1/\alpha_{n+1}] &= \frac{(\alpha_n + 1/\alpha_{n+1})\,\delta_{n-1} + \delta_{n-2}}{(\alpha_n + 1/\alpha_{n+1})\,\epsilon_{n-1} + \epsilon_{n-2}} \\ = \frac{\alpha_{n+1}\,(\alpha_n\,\delta_{n-1} + \delta_{n-2}) + \delta_{n-1}}{\alpha_{n+1}\,(\alpha_n\,\epsilon_{n-1} + \epsilon_{n-2}) + \epsilon_{n-1}} &= \frac{\alpha_{n+1}\,\delta_n + \delta_{n-1}}{\alpha_{n+1}\,\epsilon_n + \epsilon_{n-1}}.\end{aligned}$$

This can be written as an identity $M_{n+1} = M_n \cdot A_{n+1}$ for the 2×2-matrices

$$M_n := \begin{pmatrix} \delta_n & \delta_{n-1} \\ \epsilon_n & \epsilon_{n-1} \end{pmatrix}, \quad A_n := \begin{pmatrix} \alpha_n & 1 \\ 1 & 0 \end{pmatrix}.$$

The process starts with $p_0 = \alpha_0$, $q_0 = 1$ and $p_1 = \alpha_1\,\alpha_0 + 1$, $q_1 = \alpha_1$. That is, as if $M_0 = A_0$. Because $\det A_n = -1$, it follows that $\det M_n = (-1)^{n-1}$. In particular, if we take $\alpha_n = a_n \in \mathbf{Z}$, $p_n = \delta_n \in \mathbf{Z}$, $q_n = \epsilon_n \in \mathbf{Z}$ then

$$p_n\,q_{n-1} - q_n\,p_{n-1} = (-1)^{n-1}, \tag{5.5}$$

which in turn implies that $\gcd(p_n, q_n) = 1$. So $r_n = \frac{p_n}{q_n}$ is a representation of the n-th continued fraction approximation of x in the desired form. If p_{n-1}, q_{n-1}, p_n and q_n are all odd, then $p_n\,q_{n-1}$ and $q_n\,p_{n-1}$ are both even, which leads to a contradiction with (5.5). This proves (5.2).

Writing $\delta = (a_{n+1} + \xi_{n+1})\,p_n + p_{n-1}$, $\epsilon = (a_{n+1} + \xi_{n+1})\,q_n + q_{n-1}$, we have $\rho = \frac{\delta}{\epsilon}$, and we get from (5.5) that

$$\left|\frac{p_n}{q_n} - \rho\right| = \frac{1}{q_n\,\epsilon} < \frac{1}{q_n\,q_{n+1}} < \frac{1}{{q_n}^2}. \tag{5.6}$$

This proves (5.1). For the last statement, we read off from (5.5) that

$$\frac{p_n}{q_n} - \frac{p_{n-1}}{q_{n-1}} = \frac{(-1)^{n-1}}{q_{n-1}\,q_n},$$

which implies that $\frac{p_n}{q_n} > \frac{p_{n-1}}{q_{n-1}}$ if n is odd. Moreover, the absolute value of the left hand side is monotonously decreasing as a function of n. So, if n is odd, $\frac{p_{n-1}}{q_{n-1}} < \frac{p_{n+1}}{q_{n+1}} < \frac{p_n}{q_n}$ and $\frac{p_{n+1}}{q_{n+1}} < \frac{p_{n+2}}{q_{n+2}} < \frac{p_n}{q_n}$. □

We are now ready to prove:

Proposition 5.2 *There exist positive constants δ, ϵ, such that for every irrational number $\rho \in \mathbf{R}$ the following holds. Let $r_{n(j)} = \frac{p_{n(j)}}{q_{n(j)}}$ denote the j-th term in the continued fraction approximation of ρ which is not of the form odd/odd, which is an infinite sequence converging to ρ as $j \to \infty$. Then there is a sequence of points x_j such that, for all j:*

$$|x_j - \rho| \leq \delta \cdot |r_{n(j)} - \rho| \tag{5.7}$$

and, with the notation $\eta = \epsilon/\delta^{\frac{3}{4}}$:

$$|f(x_j) - f(\rho)| \geq \epsilon \cdot q_{n(j)}{}^{-\frac{1}{2}} \, |r_{n(j)} - \rho|^{\frac{1}{2}} \geq \eta \cdot |x_j - \rho|^{\frac{3}{4}}. \tag{5.8}$$

The same result holds with $f(x)$ replaced by $g(x)$. In particular, neither $f(x)$ nor $g(x)$ is differentiable at any irrational point.

Proof Let $r = r_n$ be a continued fraction approximation of ρ, of the form $r = \frac{p}{q} = \gamma^{-1}(\infty)$, $\gamma \in \Gamma_\theta$. The idea is to apply Lemma 4.3 to a suitably chosen x.

If $m = m(r)$ is even then we restrict ourselves to $x > r$ if $m = 2$ modulo 4 and to $x < r$ if $m = 0$ modulo 4, respectively, in order to ensure that x lies on the "square root side" and not on the differentiable side of r. If m is odd, then the real part of the square root term gets a factor $1/\sqrt{2}$ in front. We still have a free choice for the positive constant a in

$$|x - r| = a \cdot |r - \rho|.$$

Using (5.1), we obtain now from Lemma 4.3:

$$|f(x) - f(r)| \geq q^{-\frac{1}{2}} \cdot |r - \rho|^{\frac{1}{2}} \, a^{\frac{1}{2}} \cdot [\tfrac{1}{\sqrt{2}} - \tfrac{1}{2} a^{\frac{1}{2}} q^{-\frac{1}{2}} - \tfrac{\pi}{3} a].$$

In order to get a positive factor in the right hand side, we require that

$$0 < a < \tfrac{3}{\sqrt{2}\pi}.$$

This yields

$$|f(x) - f(r)| \geq b \, q^{-\frac{1}{2}} \cdot |r - \rho|^{\frac{1}{2}}$$

if q is sufficiently large and the constant b is chosen such that

$$0 < b < a^{\frac{1}{2}} \cdot [\tfrac{1}{\sqrt{2}} - \tfrac{\pi}{3} a].$$

We now take $r = r_{n(j)}$; in Lemma 5.1 we have seen that these form a sequence converging to ρ. Note that $|f(r) - f(\rho)|$ and $|f(x) - f(\rho)|$ are not both smaller than $\frac{1}{2}\,|f(x) - f(r)|$. So, if we take $x_j = r$ or $x_j = x$ such that $|f(x_j) - f(\rho)|$ is maximal, we get (5.8), with $\epsilon = \frac{b}{2}$. The estimate (5.7) holds with $\delta = 1 + a$ and the second estimate in (5.8) follows from (5.7) and (5.1). □

One consequence is that if a subsequence of the r_n in Proposition 5.2 satisfies $|r_n - \rho| = \mathrm{O}(q_n{}^{-\kappa})$ for some $\kappa \geq 2$, then

$$\text{not} \quad f(x) - f(\rho) = \mathrm{o}(|x - \rho|^{\frac{1}{2} + \frac{1}{2\kappa}}) \quad \text{for} \quad x \to \rho. \tag{5.9}$$

Here $v(x) = \mathrm{o}(w(x))$ means that $v(x)/w(x)$ converges to 0. In the following lemma we aim at a converse of this.

Lemma 5.3 *Suppose that the continued fraction approximations $r_n = \frac{p_n}{q_n}$ of the irrational number ρ satisfy estimates of the form*

$$|r_n - \rho| \geq \epsilon \, {q_n}^{-\kappa} \quad \textit{for all} \;\; n, \tag{5.10}$$

for some $\kappa \geq 2$, $\epsilon > 0$. Then, with the notation

$$\alpha := \alpha(\kappa) := \tfrac{3}{4}\,(1 - \kappa(\kappa - 2)),$$

we have

$$|\phi(x) - \phi(\rho)| = O(|x - \rho|^{\alpha}) \quad \textit{as} \;\; x \to \rho.$$

Proof For each $n \geq 2$, we will estimate $|\phi(x) - \phi(\rho)|$ by $C \cdot |x - \rho|^{\alpha}$, for x in the segment with endpoints r_{n-2} and r_n. According to the last statement in Lemma 5.1, these segments fill up a full punctured neighborhood of ρ. The points r_{n-2}, x, r_n and ρ lie in this order, increasing or decreasing, hence

$$|r_n - \rho| \leq |x - \rho| \leq |r_{n-2} - \rho| \quad \text{and} \quad |x - r_n| < |x - \rho|. \tag{5.11}$$

In the remainder of the proof we will use the convention that the constant C may be different at different places in the text, but at every instant depends only on κ and ϵ, and not on n.

Using Lemma 4.3 and (4.8), we get

$$\begin{aligned} |\phi(x) - \phi(\rho)| &\leq |\phi(x) - \phi(r_n)| + |\phi(r_n) - \phi(\rho)| \\ &\leq C\cdot \quad [q^{-\frac{1}{2}}\,|x - r_n|^{\frac{1}{2}} + |x - r_n| + q^{\frac{3}{2}}\,|x - r_n|^{\frac{3}{2}} \\ &\qquad + q^{-\frac{1}{2}}\,|r_n - \rho|^{\frac{1}{2}} + |r_n - \rho| + q^{\frac{3}{2}}\,|r_n - \rho|^{\frac{3}{2}}]. \end{aligned} \tag{5.12}$$

It is sufficient to majorize each term in the right hand side of (5.12) by $C \cdot |x - \rho|^{\beta}$ for some $\beta \geq \alpha$, because then it is $\mathrm{O}(|x - \rho|^{\alpha})$ for $x \to \rho$.

The second and fifth term sum to $|x - \rho|$. For the sixth term, (5.1) and (5.11) yield

$$q^{\frac{3}{2}}\,|r_n - \rho|^{\frac{3}{2}} \leq |r_n - \rho|^{-\frac{3}{4}}\,|r_n - \rho|^{\frac{3}{2}} = |r_n - \rho|^{\frac{3}{4}} \leq |x - \rho|^{\frac{3}{4}}.$$

For the fourth term, we use (5.10) and (5.11), in order to get

$$q^{-\frac{1}{2}}\,|r_n - \rho|^{\frac{1}{2}} \leq C \cdot |r_n - \rho|^{\frac{1}{2\kappa}}\,|r_n - \rho|^{\frac{1}{2}} = C \cdot |x - \rho|^{\frac{1}{2\kappa} + \frac{1}{2}}.$$

Similarly the first term is estimated by

$$q^{-\frac{1}{2}}\,|x - r_n|^{\frac{1}{2}} \leq C \cdot |r_n - \rho|^{\frac{1}{2\kappa}}\,|x - r_n|^{\frac{1}{2}} = C \cdot |x - \rho|^{\frac{1}{2\kappa} + \frac{1}{2}}.$$

For the third term we start as with the sixth term:

$$q^{\frac{3}{2}}\,|x - r_n|^{\frac{3}{2}} \leq C \cdot |r_n - \rho|^{-\frac{3}{4}}\,|x - \rho|^{\frac{3}{2}}. \tag{5.13}$$

In order to proceed further, we need that $|r_n - \rho|$ is not too small compared to $|x - \rho|$. For this, we use (5.6) together with (5.10), and get

$$|r_{n-1} - \rho| < (q_{n-1} q_n)^{-1} \leq C \cdot |r_{n-1} - \rho|^{\frac{1}{\kappa}}\,|r_n - \rho|^{\frac{1}{\kappa}},$$

which in turn implies that

$$|r_{n-1}-\rho| \leq C \cdot |r_n-\rho|^{\frac{1}{\kappa}/(1-\frac{1}{\kappa})} = C \cdot |r_n-\rho|^{\frac{1}{\kappa-1}}.$$

Combining this with the same estimate with n replaced by $n-1$, we get

$$|x-\rho| \leq |r_{n-2}-\rho| \leq C \cdot |r_n-\rho|^{(\kappa-1)^{-2}}.$$

Inserting this in (5.13), the result is that

$$q^{\frac{3}{2}}\,|x-r_n|^{\frac{3}{2}} \leq C \cdot |x-\rho|^{-\frac{3}{4}(\kappa-1)^2}\,|x-\rho|^{\frac{3}{2}}.$$

The proof is completed by observing that $\kappa \geq 2$ implies that

$$-\tfrac{3}{4}(\kappa-1)^2+\tfrac{3}{2} = \alpha \leq \tfrac{1}{2\kappa}+\tfrac{1}{2}.$$

□

The following corollary shows that the estimate (5.9) is optimal if $\kappa = 2$.

Corollary 5.4 *If the partial quotients of the continued fraction of ρ form a bounded sequence, then*

$$\phi(x)-\phi(\rho) = O(|x-\rho|^{\frac{3}{4}}) \quad as \quad x \to \rho.$$

Proof The condition just means that (5.10) holds with $\kappa = 2$, cf. (5.6), so the conclusion holds with $\alpha = \alpha(2) = \frac{3}{4}$. □

For $\kappa > 2$ there is a gap between the exponents in (5.9) and Lemma 5.3. For instance, already for $\kappa = 1+2/\sqrt{3} = 2.1547\ldots$, we have $\alpha(\kappa) = \frac{1}{2}$, and Lemma 5.3 does not give any improvement over the uniform estimate of Lemma 4.1. However, Lemma 5.3 is strong enough to conclude that for most ρ, in measure theoretic sense, we have that $\phi(x)-\phi(\rho)$ can be estimated by $|x-\rho|^\alpha$ as $x \to \rho$, for every $\alpha < \frac{3}{4}$. In order to give a concise formulation of the result, we denote the *supremum of the Hölder exponents at* ρ by

$$\alpha(\rho) := \sup\{\alpha > 0 \mid f(x)-f(\rho) = \mathrm{O}(|x-\rho|^\alpha) \ \text{ as } \ x \to \rho\}. \tag{5.14}$$

Proposition 4.5 yields that $\alpha(s) = 1$ if s is a quotient of two odd integers. The discussion after Lemma 4.3 showed that $\alpha(r) = \frac{1}{2}$ for the other rational numbers r, whereas Lemma 4.1 and Proposition 5.2 imply that $\frac{1}{2} \leq \alpha(\rho) \leq \frac{3}{4}$ if ρ is irrational. Moreover, $\alpha(\rho)$ is closer to $\frac{1}{2}$, the faster ρ can be approximated by continued fractions r such that $\alpha(r) = \frac{1}{2}$. The same conclusions hold with $f(x)$ replaced by $g(x)$. The following corollary is a sort of correction to the impression which is given by the prominent square root behaviour at rational numbers with small denominators.

Corollary 5.5 *For almost all $x \in \mathbf{R}$, we have $\alpha(x) = \frac{3}{4}$.*

Proof Because of the periodicity of ϕ, we may work modulo 2. Let G be the set of $\rho \in \mathbf{R}/2\mathbf{Z}$ which are irrational and somewhat slowly approximable by rational numbers, in the following sense. For every $\kappa > 2$ there exist an $\epsilon > 0$, such that

$$|\rho - \frac{p}{q}| \geq \epsilon \cdot q^{-\kappa} \tag{5.15}$$

holds for all integers p and all positive integers q. Although this looks like a very severe restriction, the fact is that almost every real number belongs to G, in the sense that the complement F of G in $\mathbf{R}/2\mathbf{Z}$ has zero measure. We repeat the classical argument.

Let us first fix the denominator q. The number of points $\frac{p}{q} \in \mathbf{R}/2\mathbf{Z}$, with $p \in \mathbf{Z}$, is equal to $2q$. The set $F_{q,\epsilon,\kappa}$ of $\rho \in I_l$ for which (5.15) fails for some $p \in \mathbf{Z}$ is contained in the union of the $\epsilon \cdot q^{-\kappa}$-neighborhoods of these $\frac{p}{q}$. Its measure is therefore estimated by

$$\mathrm{meas}(F_{q,\epsilon,\kappa}) \leq 2q \cdot 2\epsilon\, q^{-\kappa} \leq 4 \cdot \epsilon\, q^{1-\kappa}.$$

The set $F_{\epsilon,\kappa}$ of ρ such that (5.15) fails for some $p, q \in \mathbf{Z}$, $q > 0$, is equal to the union over all $q > 0$ of the sets $F_{q,\epsilon,\kappa}$. This yields

$$\mathrm{meas}(F_{\epsilon,\kappa}) \leq \sum_{q=1}^{\infty} 4 \cdot \epsilon\, q^{1-\kappa} = C(\kappa) \cdot \epsilon,$$

because the series $\zeta(s) = \sum_{n>0} n^{-s}$ converges if $s > 1$. The set F_κ of ρ, such that for every $\epsilon > 0$ there exist $p, q \in \mathbf{Z}$, $q > 0$, for which (5.15) fails, is contained in each $F_{\epsilon,\kappa}$. So its measure is majorized by $C(\kappa) \cdot \epsilon$. Because this holds for all $\epsilon > 0$, the conclusion is that F_κ has zero measure. The set F is equal to the union of the F_κ over all $\kappa > 2$. Because F_κ is increasing with decreasing κ, it is equal to the union of the countable sequence of sets $F_{\kappa(j)}$ where $j \mapsto \kappa(j)$ is a countable sequence which decreases to 2. Because the union of a countable sequence of sets of zero measure has zero measure, the conclusion is that F has zero measure.

If $\rho \in G$, then there exists, for every $\kappa > 2$, an $\epsilon > 0$ such that (5.10) holds. So it follows from Lemma 5.3 that $\alpha(\rho) \geq \alpha(\kappa)$. Because this holds for every $\kappa > 2$, and $\alpha(\kappa)$ converges to $\frac{3}{4}$ as $\kappa \downarrow 2$, it follows that $\alpha(\rho) \geq \frac{3}{4}$. Proposition 5.2 gave the opposite inequality for every irrational number ρ, so in fact $\alpha(\rho) = \frac{3}{4}$ for every $\rho \in G$. Again using that the union of a countable family of sets of zero measure has zero measure, we can pass from $\mathbf{R}/2\mathbf{Z}$ to $\mathbf{R}$. The conclusion is that the set of $x \in \mathbf{R}$ such that $\alpha(x) \neq \frac{3}{4}$ has zero measure. □

6 At Fixed Points

Usually the explanation for repeating patterns which converge to a point ρ is that ρ is a *fixed point* of a nontrivial element of the group which acts on the object; $,_\theta$ in our case. The following lemma shows that for rational ρ this gives back the patterns which have been observed before. We recall the notation τ_b for the translation $x \mapsto x + b$ over the integer b.

Lemma 6.1 *If $\rho \in \mathbf{Q}$ is not of the type odd/odd, then there exists a $\delta \in\, ,_\theta$ such that $\delta(\rho) = \infty$. For such δ, the element $\gamma := \delta^{-1} \circ \tau_2 \circ \delta \in\, ,_\theta$ fixes ρ. Every element of $,_\theta$ which fixes ρ is equal to an integral power of γ.*

If $\rho \in \mathbf{Q}$ is of the type odd/odd, then there exists an $\epsilon \in$, such that $\epsilon(\rho) = \infty$ and the matrix of ϵ is of the type $\begin{pmatrix} \text{odd} & \text{even} \\ \text{odd} & \text{odd} \end{pmatrix}$. For such ϵ, the element $\gamma := \epsilon^{-1} \circ \tau_1 \circ \epsilon \in$, $_\theta$ fixes ρ. Every element of , $_\theta$ which fixes ρ is equal to an integral power of γ.

Proof If $\rho \in \mathbf{Q}$ then there exists a $\epsilon \in$, such that $\epsilon(\rho) = \infty$; write $\mu := \epsilon^{-1} \circ \tau_1 \circ \epsilon$. Then $\mu(\rho) = \epsilon^{-1} \circ \tau_1(\infty) = \epsilon^{-1}(\infty) = \rho$. If conversely $\nu \in$, , $\nu(\rho) = \rho$, then $\tau := \epsilon \circ \nu \circ \epsilon^{-1}$ satisfies $\tau(\infty) = \epsilon \circ \nu(\rho) = \epsilon(\rho) = \infty$. In the discussion in front of Lemma 3.2 we have seen that this implies that τ is equal to a translation over an integer b. That is, $\tau = {\tau_1}^b$, which in turn implies that $\nu = \mu^b$.

If ρ is not of the type odd/odd, then we can take $\epsilon \in$, $_\theta$ and then $\gamma := \mu^2 \in$, $_\theta$. Also, $\tau \in$, $_\theta$, or b is even, which means that ν is equal to an integral power of γ.

Finally, if ρ is of the type odd/odd, then the bottom row of the matrix of ϵ is of the type odd, odd. If the top row is of the type even, odd, then by adding the bottom row to it we can change ϵ into an element of , of the desired type, without altering the pole point ρ. If the matrix of ϵ is of the type $\begin{pmatrix} \text{odd} & \text{even} \\ \text{odd} & \text{odd} \end{pmatrix}$, then the matrix of γ is of the type $\begin{pmatrix} \text{even} & \text{odd} \\ \text{odd} & \text{even} \end{pmatrix}$. We conclude from Lemma 3.2 that $\gamma \in$, $_\theta$. □

For any $\rho \in \mathbf{R}$, $\gamma : x \mapsto \frac{ax+b}{cx+d} \in$, $_\theta$, the equation $\gamma(\rho) = \rho$ is equivalent to

$$c \cdot \rho^2 + (d - a) \cdot \rho - b = 0. \tag{6.1}$$

With the notation $t = \frac{a+d}{2} \in \mathbf{Z}$, we can read off ρ and $\gamma'(\rho) = (c\,\rho + d)^{-2}$ from

$$c\,\rho + d = t \pm \sqrt{t^2 - 1}. \tag{6.2}$$

Because the matrix of a translation has trace equal to 2 and the trace is invariant under conjugation, it follows from Lemma 6.1 that $t = 1$ if $\rho \in \mathbf{Q}$. Conversely $t = 1$ implies that $\rho = \frac{1-d}{c} \in \mathbf{Q}$. Also, $\gamma'(\rho) = 1$ in this case, which implies that $\gamma^j(x)$ converges very slowly to ρ as $j \to \pm\infty$. More precisely, Lemma 6.1 tells that there exist $\epsilon \in$, , $k \in \mathbf{Z}$ such that $\gamma^j(x) = \epsilon^{-1}(\epsilon(x) + j \cdot k)$, so the convergence is of the order $\mathrm{O}(\frac{1}{j})$ and the selfsimilarity at ρ is identical to the one explained in front of Figure 4.2. A similar explanation can be given for the selfsimilarities at the rational points of type odd/odd.

We now turn to the irrational fixed points of elements of , $_\theta$. In the following classification, a *quadratic surd* is defined as an irrational solution ρ of an equation $A\,\rho^2 + B\,\rho + C = 0$, with $A, B, C \in \mathbf{Z}$, $A \neq 0$. One says that the irrational number ρ has a *periodic continued fraction* if there exist integers $\omega > 0$ and $j \geq 0$ such that the partial quotients a_n of the continued fraction of ρ satisfy $a_{n+\omega} = a_n$ for all $n \geq j$.

Lemma 6.2 *The following conditions (a)-(c) for the real number ρ are equivalent.*

(a) ρ is fixed by some $\gamma \in$, $_\theta$ such that $0 < \gamma'(\rho) < 1$.

(b) ρ is a quadratic surd.

(c) The continued fraction of ρ is periodic.

All elements of , $_\theta$ which fix ρ are integral powers of one of these.

Proof If (a) holds then it follows from the discussion after Lemma 6.1 that ρ is irrational, so (b) follows from (6.1). For the implication (b) $\Rightarrow$ (c) we refer to Hardy and Wright [10, Section 10.12, Theorem 177].

Now assume that the continued fraction of ρ is periodic. In terms of the matrices

$$M_n := \begin{pmatrix} p_n & p_{n-1} \\ q_n & q_{n-1} \end{pmatrix}, \quad A_n := \begin{pmatrix} a_n & 1 \\ 1 & 0 \end{pmatrix},$$

for which $M_n = M_{n-1} \cdot A_n$, see the proof of Lemma 5.1, this means that $A_{n+\omega} = A_n$ for all $n \geq j$. Hence $M_{n+\omega} \cdot {M_n}^{-1} = M_{n+\omega-1} \cdot {M_{n-1}}^{-1}$, or

$$M_{n+\omega} \cdot {M_n}^{-1} = B := M_{j+\omega-1} \cdot {M_{j-1}}^{-1} = M_{j-1} \cdot A_j \cdot \ldots \cdot A_{j+\omega-1} \cdot {M_{j-1}}^{-1} \quad \text{for all} \quad n \geq j.$$

Or, $M_{n+\omega} = B \cdot M_n$, which in turn implies that $M_{n+k\omega} = B^k \cdot M_n$ for all $n \geq j,\ k > 0$.

From this it follows that the line through the column vector

$$\begin{pmatrix} p_{n+k\omega} \\ q_{n+k\omega} \end{pmatrix}$$

converges for $k \to \infty$ to an eigenspace of B. In view of the interpretation of the fractional linear transformation β with matrix B as the action of B on the projective line, this means that the limit ρ, for $k \to \infty$, of the $p_{n+k\omega}/q_{n+k\omega}$, is a fixed point of β.

If $\det B = -1$, then one may pass to $\beta^2 \in$, , of which ρ is a fixed point as well. Because for every $\alpha \in$, we have that α, α^2, or α^3 belongs to , $_\theta$, we get that some power γ of β belongs to , $_\theta$. The proof of (c) $\Rightarrow$ (a) is complete if we can arrange that $\gamma'(\rho) < 1$, note that always $\gamma'(\rho) > 0$.

γ is not equal to the identity, because if $B^k = 1$, $k > 0$, then $M_{n+k\omega} = M_n$, in contradiciton with the convergence behaviour of the $\frac{p_n}{q_n}$ towards ρ. It follows from (6.2), $\rho \notin \mathbf{Q}$, that $\gamma'(\rho) \neq 1$. If $\gamma'(\rho) > 1$ then we replace γ by γ^{-1}, which fixes ρ as well, and has derivative at ρ equal to $1/\gamma'(\rho) < 1$.

For the last statement we observe that if $\rho \notin \mathbf{Q}$, then 1, ρ and ρ^2 span a 2-dimensional vector space over $\mathbf{Q}$. This implies that if $A\,\rho^2 + B\,\rho + C = 0$ and $A'\,\rho^2 + B'\,\rho + C' = 0$, with $A, B, C, A', B', C' \in \mathbf{Z}$, $A \neq 0$, then there exists $\theta \in \mathbf{Q}$ such that $A' = \theta\,A$, $B' = \theta\,B$, $C' = \theta\,C$. That is, all quadratic equations with integral coefficients of which ρ is a solution, have the same other solution ρ'. It follows that if A is the matrix of an element of , $_\theta$ which fixes ρ, then

$$L := R^{-1} \cdot A \cdot R = \begin{pmatrix} \lambda & 0 \\ 0 & \mu \end{pmatrix}, \quad \text{for} \qquad R := \begin{pmatrix} \rho & \rho' \\ 1 & 1 \end{pmatrix}.$$

Here R is independent of A. Furthermore, $\det L = \det A = 1$, hence $\mu = 1/\lambda$. Because A is determined up to multiplication by -1, we may assume that $\lambda > 0$.

The elements of , $_\theta$ which fix ρ form a group, so the λ which we get form a multiplicative subgroup Λ of $\mathbf{R}_{>0}$. On the other hand it follows from $\lambda + \frac{1}{\lambda} = \operatorname{trace}(L) = \operatorname{trace}(A) \in \mathbf{Z}$ that Λ is a discrete subset of $\mathbf{R}_{>0}$. The proof is completed by the observation that a discrete nontrivial subgroup Λ of $\mathbf{R}_{>0}$ consists of the integral powers of the smallest $\lambda \in \Lambda$ such that $\lambda > 1$. Using the substitution of variables $\lambda = \exp(x)$, this is equivalent to the more familiar fact that a discrete nontrivial additive subgroup P of $\mathbf{R}$ is of the form $P = \mathbf{Z} \cdot p$, where p is the smallest positive element of P. $\square$

Now let ρ satisfy any of the equivalent conditions (a)-(c) in Lemma 6.2. Because the sequence of partial fractions of a periodic continued fraction is bounded, we see from Corollary 5.4 that $\phi(x)-\phi(\rho)$ has exactly the order $|x-\rho|^{\frac{3}{4}}$ as $x \to \rho$. However, the fixed point property shows this even more directly and in a stronger form, as we shall explain now.

Because $0 < \gamma'(\rho) < 1$ we get, near ρ, that the iterates of γ contract exponentially towards ρ in the sense that

$$\gamma^j(x) - \rho = \mathrm{O}(|\gamma'(\rho)|^j) \tag{6.3}$$

as $j \to \infty$, locally uniformly for x near ρ. The equation (4.1) now leads to a selfsimilarity near ρ, which however is very different in nature from the one near the rational points, because the patterns repeat themselves in a *geometric progression* towards ρ. This faster convergence makes that in enlargements around these ρ one sees much fewer repeated patterns than near the rational points. The selfsimilarity can be written in the form $\phi(x) = \lambda(x) \cdot \phi(\gamma(x)) + \beta(x)$, with λ and β of class $C^{1,\frac{1}{2}}$ near ρ, and

$$\lambda(x) = e^{\frac{\pi i}{4}m} \cdot q^{\frac{3}{2}}\,(x-r)^{\frac{3}{2}}.$$

Because $\gamma'(\rho) = q^{-2}\,(\rho - r)^{-2}$, we see that $|\lambda(\rho)| = |\gamma'(\rho)|^{-\frac{3}{4}}$. This implies that $\phi(x) - \phi(\rho)$ has exactly the order $|x-\rho|^{\frac{3}{4}}$ as $x \to \rho$. The factor $e^{\frac{\pi i}{4}m}$ makes that it may take several iterates of γ before we get a similarity of the real part $f(x)$ of $\phi(x)$. For instance, if m is odd, then one gets the similarity, with a reflection in the vertical direction, only after 4 iterates.

Actually, one needs very good eyes to see the selfsimilarities at the fixed points directly in the graph of $f(x)$. Taking m even means in view of (3.9) that c is even and d is odd. The condition that $\gamma \in \Gamma_\theta$ then forces that a is odd and b is even, cf. Lemma 3.2. If t is even then, *modulo 4*, we have $1 = ad - bc = -d^2 = -1$, a contradiction. This leads to the conclusion that $\gamma'(\rho)$ is closest to 1 if $t = \pm 3$, in which case

$$\gamma'(\rho) = 17 - 12\sqrt{2} = \tfrac{1}{17+12\sqrt{2}} \approx \tfrac{1}{33.97}.$$

After a few enlargements with this factor, one needs so many terms in the series (1.1) in order to get a decent relative accuracy, that, even with a fast computer, it becomes quite time-consuming to get a sharp picture.

Figures 6.1 and 6.2 illustrate $f(x)$ near $x = \rho := 1 + \sqrt{2}$, which is the fixed point ρ of $\gamma : x \mapsto \frac{5x+2}{2x+1}$ where $\gamma'(\rho) < 1$. The pole point is $r = \frac{-1}{2}$, so $m = 0$, cf. Table 4.4. Because of the steepness of $f(x)$, we have compressed the first picture in the vertical direction by a factor of 3. The axes are $x = \rho$ and $y = f(\rho)$. The window is the outline of the next enlargement. The x-size is multiplied by $\gamma'(\rho) = 17 - 12\sqrt{2}$, the y-size by $\gamma'(\rho)^{\frac{3}{4}}$. For the second picture we have performed an additional compression in the vertical direction in order to get it in the same frame as the first picture.

$|x| < 0.0477$
$|y| < 0.0358$

Figure 6.1: $y = \frac{1}{3}\,(f(\rho + x) - f(\rho)), \quad \rho = 1 + \sqrt{2}$

$|x| < 0.00141$
$|y| < 0.00105$

Figure 6.2: $y = 0.138\,(f(\rho + x) - f(\rho)), \quad \rho = 1 + \sqrt{2}$

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