New Integral Representations for the Square of the Riemann Zeta-function

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Introduction

The recent discovery of an analogue of the Riemann-Siegel integral formula for Dirichlet series associated to cusp forms [2] naturally arises the question whether similar formulas might exist for other types of zeta functions. The proof of these formulas merely depends on the functional equation for the underlying Dirichlet series. In both cases, for $\zeta(s)$ and for the cusp form zeta functions, only a simple gamma factor is involved. The next simplest case arises when two such factors occur in the functional equation. The prototype of these Dirichlet series is $\zeta^2(s)$, and so any investigation might well begin with this example. In the present study we show that, indeed, a formula of Riemann-Siegel type can be found for $\zeta^2(s)$.

The numerous applications of the ordinary Riemann-Siegel integral formula [3] suggest similar ones for our formula too. For instance, it seems very probable to derive an asymptotic expansion for $\zeta^2(s)$, giving a generalization of Siegel's result [9]. Originally, this expansion is due to Motohashi [6, 7], and it depends on the corresponding formula for $\zeta(s)$. Consequently, our approach might lead to an independent proof of Motohashi's expansion. This would be of considerable value, since our method applies as well to other Dirichlet series satisfying similar functional equations, like Hecke L series of quadratic fields. As a first step in this direction we give a simple proof of the approximate functional equation for $\zeta^2(s)$ at the end of the paper.

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1. Basic Formulas

Let $s = \sigma + it$, σ, t real, and $R(s) = \pi^{-\frac{s}{2}}\Gamma(\frac{s}{2})\zeta(s)$. From well known properties of the zeta function [3] it follows that R has simple poles at $s = 1$ and $s = 0$ with residues being equal to 1 and $2\zeta(0) = -1$ respectively, and otherwise is regular. Moreover, R satisfies the functional equation $R(s) = R(1-s)$. For $c > 1$, $x > 0$ consider

$$\psi(x) = \frac{1}{2\pi i}\int_{(c)} R^2(s)x^{-s}\mathrm{d}s = \frac{1}{2\pi i}\int_{(c)} \pi^{-s}\Gamma^2\left(\frac{s}{2}\right)\zeta^2(s)x^{-s}\mathrm{d}s. \tag{1.1}$$

Inserting the series $\sum_{n=1}^{\infty} d(n)n^{-s}$ for $\zeta^2(s)$ and interchanging the order of integration and summation, which is permitted by absolute convergence, yields

$$\psi(x) = \sum_{n=1}^{\infty} d(n)\frac{1}{2\pi i}\int_{(c)} \Gamma^2\left(\frac{s}{2}\right)(\pi n x)^{-s}\mathrm{d}s.$$

The integral is equal to $8\pi i K_0(2\pi n x)$, where K_0 denotes the usual modified Bessel function, in view of the Mellin transform [5, p.14]

$$\frac{1}{2\pi i}\int_{(c)} \Gamma^2\left(\frac{s}{2}\right)\left(\frac{y}{2}\right)^{-s}\mathrm{d}s = 4K_0(y).$$

Hence

$$\psi(x) = 4\sum_{n=1}^{\infty} d(n)K_0(2\pi n x). \tag{1.2}$$

The asymptotic relation $K_0(y) = O(y^{-\frac{1}{2}}e^{-y})$, valid for $y \to \infty$ in the sector $|\arg(y)| < \frac{3\pi}{2}$, shows that the series (1.2) converges absolutely and uniformly in any half plane $\mathrm{Re}(x) \geq \delta > 0$. It follows that (1.2) defines a function ψ holomorphic in the right half plane $\mathrm{Re}(x) > 0$. The imaginary axis is a natural boundary for ψ. This fact can, for instance, easily be deduced from Lemma 2 below. In the sequel it will turn out that ψ is the basic function on whose properties most of our results depend. It is therefore necessary to investigate it more closely. Obviously, ψ is related to the Eisenstein series $E_0(z)$ [4]. Contrary to the usual use of this non-analytic function, where E_0 is considered as a function of the real variables x, y (where $z = x + iy$), it is here the behaviour for complex values of y that matters.

Next we derive a functional equation for ψ. To this end the line $\mathrm{Re}(s) = c > 1$ of integration in (1.1) is shifted to $\mathrm{Re}(s) = \frac{1}{2}$. The integrand has a pole of order 2 at $s = 1$ with residue being equal to

$$r(x) = \frac{1}{x}\log\frac{1}{x} + \frac{1}{x}(\gamma - \log\pi - 2\log 2), \tag{1.3}$$

using $(\Gamma'/\Gamma)(\frac{1}{2}) = -\gamma - 2\log 2$, where γ denotes Euler's constant. Thus

$$\psi(x) = r(x) + \frac{1}{2\pi i}\int_{(\frac{1}{2})} R^2(s)x^{-s}\mathrm{d}s = r(x) + \frac{1}{2\pi i}\int_{(\frac{1}{2})} R^2(1-s)x^{-s}\mathrm{d}s.$$

The last integral is easily transformed into

$$\frac{1}{2\pi i}\int_{(\frac{1}{2})} R^2(w)x^{w-1}\mathrm{d}w = -\frac{1}{x}r\left(\frac{1}{x}\right) + \frac{1}{2\pi i x}\int_{(\frac{3}{2})} R^2(w)x^{w}\mathrm{d}w = -\frac{1}{x}r\left(\frac{1}{x}\right) + \frac{1}{x}\psi\left(\frac{1}{x}\right).$$

Therefore we have the functional equation for ψ,

$$\psi(x) = r(x) - \frac{1}{x}r\left(\frac{1}{x}\right) + \frac{1}{x}\psi\left(\frac{1}{x}\right), \tag{1.4}$$

valid throughout the half plane $\mathrm{Re}(x) > 0$.

We are now going to derive new integral formulas for $\zeta^2(s)$. Our starting point is the representation

$$R^2(s) = \int_0^\infty \psi(x)x^{s-1}\mathrm{d}x, \quad \sigma > 1, \tag{1.5}$$

obtained by inverting (1.1).

Lemma 1: *In the plane cut from 0 to $-\infty$ we have*

$$K_0(z) = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} e^{-z}\left[1 + H(z)\right],$$

where H is holomorphic and the principal branch of the square root is taken. If $\mathrm{Re}(z) \geq 0$, $z \neq 0$, *we have* $|H(z)| \leq 2$, *and if in addition* $|z| \geq 1$, *then* $|H(z)| \leq |z|^{-1}$.

Proof: We apply the formula [5, p.119]

$$K_0(z) = \int_1^\infty e^{-zt}(t^2-1)^{-\frac{1}{2}}\mathrm{d}t, \quad \mathrm{Re}(z) > 0.$$

The substitution $t = 1 + \frac{x}{z}$ gives

$$K_0(z) = (2z)^{-\frac{1}{2}}e^{-z}\int_0^\infty e^{-x}x^{-\frac{1}{2}}\left(1 + \frac{x}{2z}\right)^{-\frac{1}{2}}\mathrm{d}x.$$

By analytic continuation, this formula extends to the entire z plane cut from 0 to $-\infty$. With the principal branch of the argument we have $-\pi < \arg(z) < \pi$. Write the above formula in the form

$$K_0(z) = (2z)^{-\frac{1}{2}} e^{-z} \left\{ \int_0^\infty e^{-x} x^{-\frac{1}{2}} \mathrm{d}x + \int_0^\infty e^{-x} x^{-\frac{1}{2}} h\left(\frac{x}{2z}\right) \mathrm{d}x \right\},$$

where $h(w) = (1+w)^{-\frac{1}{2}} - 1$. Since

$$h(w) = \frac{1-\sqrt{1+w}}{\sqrt{1+w}} = \frac{-w}{\sqrt{1+w}+1+w},$$

we get immediately $|h(w)| \leq \frac{1}{2}|w|$ and $|h(w)| \leq 2$, provided $\mathrm{Re}(w) \geq 0$. Thus, defining

$$H(z) = \pi^{-\frac{1}{2}} \int_0^\infty e^{-x} x^{-\frac{1}{2}} h\left(\frac{x}{2z}\right) \mathrm{d}x = \pi^{-\frac{1}{2}} \int_0^\infty e^{-x} x^{-\frac{1}{2}} \left[\left(1+\frac{x}{2z}\right)^{-\frac{1}{2}} - 1\right] \mathrm{d}x,$$

we see that the first assertion is true. Let $z \neq 0$, $\mathrm{Re}(z) \geq 0$. Splitting the last integral at $|z|$ and applying the above inequalities to $h(\frac{x}{2z})$ leads to

$$\begin{aligned} \pi^{\frac{1}{2}} |H(z)| &\leq \frac{1}{4}|z|^{-1} \int_0^{|z|} e^{-x} x^{\frac{1}{2}} \mathrm{d}x + 2\int_{|z|}^\infty e^{-x} x^{-\frac{1}{2}} \mathrm{d}x \\ &< \frac{1}{4}|z|^{-1} \Gamma\left(\frac{3}{2}\right) + 2|z|^{-\frac{1}{2}} e^{-|z|} = |z|^{-1}\left(\frac{1}{8}\sqrt{\pi} + 2|z|^{\frac{1}{2}} e^{-|z|}\right). \end{aligned}$$

The expression in parantheses is less than 1 if $|z| \geq 1$, thereby proving the last assertion. Concerning the second one, we simply use $|h(\frac{x}{2z})| \leq 2$ for $\mathrm{Re}(z) \geq 0$, $z \neq 0$. Then

$$|H(z)| \leq 2\pi^{-\frac{1}{2}} \int_0^\infty e^{-x} x^{-\frac{1}{2}} \mathrm{d}x = 2\pi^{-\frac{1}{2}} \Gamma\left(\frac{1}{2}\right) = 2.$$

This concludes the proof of Lemma 1.

Lemma 2: *Let* $\mathrm{Re}(x) > 0$. *Then the function* $\psi(x) = 4\sum_{n=1}^\infty d(n) K_0(2\pi n x)$ *admits a decomposition*

$$\psi(x) = 2x^{-\frac{1}{2}} \left[F(x) + F_1(x)\right],$$

where F, F_1 *are analytic in the half plane* $\mathrm{Re}(x) > 0$, *and where the principal branch of the square root is taken. Moreover,* F_1 *is continuous in* $\mathrm{Re}(x) \geq 0$, $x \neq 0$, *and* F *is explicitly given by*

$$F(x) = \sum_{n=1}^\infty d(n) n^{-\frac{1}{2}} e^{-2\pi n x}, \quad \mathrm{Re}(x) > 0. \tag{1.6}$$

Proof: Using Lemma 1 with $z = 2\pi n x$ gives for $\mathrm{Re}(x) > 0$

$$\begin{aligned} \psi(x) &= 2x^{-\frac{1}{2}} \sum_{n=1}^\infty d(n) n^{-\frac{1}{2}} e^{-2\pi n x} \left[1 + H(2\pi n x)\right] = 2x^{-\frac{1}{2}} \left[F(x) + F_1(x)\right], \\ F_1(x) &= \sum_{n=1}^\infty d(n) n^{-\frac{1}{2}} e^{-2\pi n x} H(2\pi n x). \end{aligned} \tag{1.7}$$

The infinite series defining $F(x)$ and $F_1(x)$ for $\mathrm{Re}(x) > 0$ are absolutely and uniformly convergent in any half plane $\mathrm{Re}(x) \geq \delta > 0$. Hence F, F_1 are analytic in $\mathrm{Re}(x) > 0$.

It remains to prove that F_1 is continuous for $\mathrm{Re}(x) \geq 0$, $x \neq 0$. Let ε be given, $0 < \varepsilon \leq \frac{1}{2}$, and assume $|x| \geq \varepsilon$. We show that the series (1.7) converges uniformly. Define an integer N by $N = 1 + [(2\pi\varepsilon)^{-1}]$. If $n > N$ then $|2\pi nx| > 2\pi N|x| \geq 2\pi N\varepsilon > 1$. Thus $|H(2\pi nx)| \leq |2\pi nx|^{-1}$ by Lemma 1. Since $|H(2\pi nx)| \leq 2$ always, we get

$$\Big|\sum_{n=1}^{\infty} d(n)n^{-\frac{1}{2}}e^{-2\pi nx}H(2\pi nx)\Big| \leq 2\sum_{n\leq N} d(n)n^{-\frac{1}{2}} + |2\pi x|^{-1}\sum_{n>N} d(n)n^{-\frac{3}{2}}$$
$$\ll N^{\frac{1}{2}}\log N + |x|^{-1} \ll \varepsilon^{-\frac{1}{2}}|\log\varepsilon| + \varepsilon^{-1} \ll \varepsilon^{-1},$$

using well known estimates for the divisor function. This completes the proof of the lemma.

Next we want to study the behaviour of $\psi(x)$ as $\mathrm{Re}(x) \to 0$, which is crucial to our investigation. As it will turn out, we can obtain very precise approximations for $\psi(x)$ if x approaches the "cusps" $i\frac{p}{q}$, p, q integers, $q > 0$, on the imaginary axis. In this way $\psi(x)$ resembles properties of modular functions, despite the fact that it is not a modular function. Lemma 2 shows that we are reduced to an investigation of $F(x) = \sum_{n=1}^{\infty} d(n)n^{-\frac{1}{2}}e^{-2\pi nx}$ for $\mathrm{Re}(x) \to 0^+$, since $F_1(x)$ is continuous on the imaginary axis ($x \neq 0$). To accomplish the desired task, we need to introduce the Dirichlet series

$$D(s, \xi_q^p) = \sum_{n=1}^{\infty} d(n)\xi_q^{np}n^{-s}, \quad \xi_q = e^{\frac{2\pi i}{q}}, \quad \sigma > 1. \tag{1.8}$$

These functions have already been studied by Estermann [1] in a classical work, from which we borrow those results relevant to our problem. Thus let p, q be integers, $q > 0$ and $(p, q) = 1$. Clearly, $D(s, \xi_q^p)$ as given by (1.8), is analytic for $\sigma > 1$. Moreover, as Estermann has shown [1, Sections 3, 4], D can be analytically continued to the entire plane where it is holomorphic, except for a double pole at $s = 1$ with residue $\frac{2}{q}(\gamma - \log q)$. More precisely, for $|\delta| < 1$

$$D(1+\delta, \xi_q^p) = \frac{1}{q}\big[\delta^{-2} + 2(\gamma - \log q)\delta^{-1} + O(1)\big]. \tag{1.9}$$

The significance of the parameters p and q can best be seen from the approximate functional equation for $\zeta^2(s)$. When $p = q = 1$, the "symmetric" form is obtained, while other choices lead to an "unsymmetric" form, as given by Motohashi [6, III]. Compare also the remarks at the end of the paper.

We now prove

Lemma 3: *Let p, q be fixed integers, $q > 0$, $(p, q) = 1$, x complex with $\mathrm{Re}(x) > 0$, and let δ_0 be a real number, $0 \leq \delta_0 < \frac{\pi}{2}$. Then*

$$F\left(i\frac{p}{q} + x\right) = (2x)^{-\frac{1}{2}}q^{-1}(\gamma - 2\log 2 - 2\log q - \log 2\pi x) + D\left(\frac{1}{2}, \xi_q^{-p}\right) + O\big(|x|^{\frac{1}{2}}\big)$$

for $x \to 0$ uniformly in the sector $|\arg(x)| \leq \delta_0$.

Proof: We have $F(i\frac{p}{q} + x) = \sum_{n=1}^{\infty} d(n)\xi_q^{-np}n^{-\frac{1}{2}}e^{-2\pi nx}$. Using Mellin's integral for $e^{-2\pi nx}$ we find for any $c > \frac{1}{2}$

$$F\left(i\frac{p}{q} + x\right) = \frac{1}{2\pi i}\int_{(c)} \Gamma(w)D\left(w + \frac{1}{2}, \xi_q^{-p}\right)(2\pi x)^{-w}\mathrm{d}w.$$

Shifting the integral to the left to the line $\mathrm{Re}(w) = -\frac{1}{2}$ and allowing for the poles at $w = \frac{1}{2}$ and $w = 0$ shows

$$F\left(i\frac{p}{q} + x\right) = \frac{1}{q\sqrt{2x}}(\gamma - 2\log 2 - 2\log q - \log 2\pi x) + D\left(\frac{1}{2}, \xi_q^{-p}\right) +$$
$$+ \frac{(2\pi x)^{\frac{1}{2}}}{2\pi i}\int_{(0)} \Gamma\left(s - \frac{1}{2}\right)D(s, \xi_q^{-p})(2\pi x)^{-s}\mathrm{d}s.$$

The residue at $w = \frac{1}{2}$ is easily calculated using (1.9). Since $D(it, \xi_q^{-p}) \ll t^A$ for some constant A, it follows from Stirling's formula and $|x^{-s}| = |x^{-it}| = e^{t\arg(x)} \le e^{\delta_0|t|}$, that the last integral is absolutely and uniformly convergent. This completes the proof of Lemma 3.

Our last preparatory result is

Lemma 4: *Let ξ be a complex number such that $0 \le \arg(\xi) < \frac{\pi}{2}$. Then for all complex $s \ne 0, 1$*

$$R^2(s) = \int_{\xi}^{\xi+\infty} \psi(x)x^{s-1}\mathrm{d}x + \int_{\xi^{-1}}^{\xi^{-1}+\infty} \psi(x)x^{-s}\mathrm{d}x + H(s,\xi),$$

with the meromorphic function

$$H(s,\xi) = \frac{\xi^{s-1}}{s-1}\left(-\log\xi + \frac{1}{s-1} + \gamma - 2\log 2 - \log\pi\right) - \\ - \frac{\xi^s}{s}\left(\log\xi - \frac{1}{s} + \gamma - 2\log 2 - \log\pi\right).$$

Proof: Assume $\sigma > 1$ and let $\delta = \arg(\xi)$. Then $0 \le \delta < \frac{\pi}{2}$ by assumption. Since $\psi(x)$ is holomorphic in $\mathrm{Re}(x) > 0$ and vanishes exponentially for $x \to \infty$ in the sector $|\arg(x)| \le \delta$, we may turn the line of integration in (1.5) about the origin. Hence

$$R^2(s) = \int_0^{e^{i\delta}\infty} \psi(x)x^{s-1}\mathrm{d}x, \quad \sigma > 1.$$

The restriction $\sigma > 1$ will be maintained for the time being. Now split the integral at $x = \xi$ and apply the functional equation (1.4) to the path from 0 to ξ. This leads, after a substitution $x \to x^{-1}$, to the formula

$$R^2(s) = \int_{\xi}^{\xi\infty} \psi(x)x^{s-1}\mathrm{d}x + \int_{\xi^{-1}}^{\xi^{-1}\infty} \psi(x)x^{-s}\mathrm{d}x + H(s,\xi),$$

where

$$H(s,\xi) = \int_0^{\xi} \left[r(x) - \frac{1}{x}r\left(\frac{1}{x}\right)\right] x^{s-1}\mathrm{d}x.$$

Here $H(s,\xi)$ can be calculated explicitly using $r(x) = \frac{1}{x}\log\frac{1}{x} + \frac{1}{x}(\gamma - \log\pi - 2\log 2)$ and

$$\int_0^{\xi} x^{w-1}\log x\mathrm{d}x = \frac{\mathrm{d}}{\mathrm{d}w}\int_0^{\xi} x^{w-1}\mathrm{d}x = \frac{\xi^w}{w}\left(\log\xi - \frac{1}{w}\right).$$

This yields the stated formula for $H(s,\xi)$ if $\sigma > 1$. Analytic continuation provides the validity of our assertion for all complex $s \ne 0, 1$ (which are poles of H). Finally we note that the integrals above can be turned about $-\delta$ and δ, respectively, so as to run parallel to the positive real axis. This concludes the proof of the lemma.

We can now state our first main theorem:

Theorem 1: *Let p, q be positive integers, $(p,q) = 1$, and δ be real, $0 \le \delta < \frac{\pi}{2}$, $\xi = \frac{p}{q}e^{i\delta}$. For complex s define*

$$T_0(s,\xi) = \int_{\xi}^{\xi+\infty} \psi(x)x^{s-1}\mathrm{d}x.$$

Then the limit $\lim_{\delta\to\pi/2} T_0(s,\xi)$ *exists, i.e.*

$$T_0\left(s, i\frac{p}{q}\right) = \int_{i\frac{p}{q}}^{i\frac{p}{q}+\infty} \psi(x)x^{s-1}\mathrm{d}x.$$

Proof: Let $\delta = \frac{\pi}{2} - \varepsilon$, so that $0 < \varepsilon \le \frac{\pi}{2}$ and $\xi = \frac{p}{q}e^{i(\frac{\pi}{2}-\varepsilon)} = i\frac{p}{q}e^{-i\varepsilon}$. Then $\delta \to \frac{\pi}{2}$ is equivalent to $\varepsilon \to 0$ and $\xi \to i\frac{p}{q}$. Moreover, we define w by $\xi = i\frac{p}{q} + w$. Then $w = \frac{p}{q}\big(\sin\varepsilon + i(\cos\varepsilon - 1)\big)$. Thus for $\varepsilon \to 0$

$$|w| = \frac{p}{q}\varepsilon + O(\varepsilon^2), \quad \arg(w) = -\frac{\varepsilon}{2} + O(\varepsilon^2). \tag{1.10}$$

Now consider the integral defining $T_0(s,\xi)$, which we may write as

$$T_0(s,\xi) = \int_w^{w+\infty} \psi\left(i\frac{p}{q}+x\right)\left(i\frac{p}{q}+x\right)^{s-1}\mathrm{d}x. \tag{1.11}$$

We apply the decomposition of $\psi(x)$ as given by Lemma 2. We get

$$T_0(s,\xi) = 2\int_w^{w+\infty} F\left(i\frac{p}{q}+x\right)\left(i\frac{p}{q}+x\right)^{s-\frac{3}{2}}\mathrm{d}x + 2\int_w^{w+\infty} F_1\left(i\frac{p}{q}+x\right)\left(i\frac{p}{q}+x\right)^{s-\frac{3}{2}}\mathrm{d}x.$$

Since F_1 is continuous for $\mathrm{Re}(x) \ge 0$, $x \ne 0$, the second integral exists if $w \to 0$. As to the first, it suffices to consider $\int_w^{w+1} F(i\frac{p}{q}+x)(i\frac{p}{q}+x)^{s-3/2}\mathrm{d}x$ for $w \to 0$. Write $x = w + u$, $0 \le u \le 1$. If ε is small enough, $|\arg(w)| \le \frac{\pi}{4}$ (say) by (1.10). Hence Lemma 3 applies. Accordingly there exist complex numbers a, b, such that $F(i\frac{p}{q}+x) = x^{-\frac{1}{2}}(a\log x + b) + O(1)$. Therefore

$$\int_w^{w+1} F\left(i\frac{p}{q}+x\right)\left(i\frac{p}{q}+x\right)^{s-\frac{3}{2}}\mathrm{d}x = \int_w^{w+1}\left[x^{-\frac{1}{2}}(a\log x + b) + O(1)\right]\left(i\frac{p}{q}+x\right)^{s-\frac{3}{2}}\mathrm{d}x.$$

The last integral converges for $w \to 0$. Thus the limit $w \to 0$ ($\xi \to i\frac{p}{q}$) in (1.11) exists too and the proof of the theorem is completed.

It is now easy to express $\zeta^2(s)$ in terms of $T_0(s, i\frac{p}{q})$:

Theorem 2: *Let p, q be positive integers, $(p,q) = 1$. Then for $s \ne 0, 1$*

$$\zeta^2(s) = T\left(s, \frac{p}{q}\right) + X(s)\overline{T\left(1-\overline{s}, \frac{q}{p}\right)} + \pi^s\Gamma^{-2}\left(\frac{s}{2}\right)H\left(s, i\frac{p}{q}\right),$$

where

$$T\left(s, \frac{p}{q}\right) = \pi^s\Gamma^{-2}\left(\frac{s}{2}\right)\int_{i\frac{p}{q}}^{i\frac{p}{q}+\infty} \psi(x)x^{s-1}\mathrm{d}x, \quad X(s) = \pi^{2s-1}\frac{\Gamma^2(\frac{1-s}{2})}{\Gamma^2(\frac{s}{2})},$$

and

$$H\left(s, i\frac{p}{q}\right) = \left(\frac{p}{q}\right)^{s-1}\frac{e^{\frac{\pi i}{2}(s-1)}}{s-1}\left(-\frac{\pi i}{2} - \log\frac{p}{q} + \frac{1}{s-1} + \gamma - 2\log 2 - \log\pi\right) -$$
$$-\left(\frac{p}{q}\right)^{s}\frac{e^{\frac{\pi i s}{2}}}{s}\left(\frac{\pi i}{2} + \log\frac{p}{q} - \frac{1}{s} + \gamma - 2\log 2 - \log\pi\right).$$

Proof: Let $\xi = \frac{p}{q}e^{i\delta}$, where $0 \le \delta < \frac{\pi}{2}$. By Lemma 4 and Theorem 1

$$R^2(s) = T_0(s,\xi) + T_0(1-s,\xi^{-1}) + H(s,\xi).$$

From $\overline{T_0(s,\xi)} = T_0(\overline{s},\overline{\xi})$ we get

$$T_0(1-s,\xi^{-1}) = \overline{T_0(1-\overline{s},\overline{\xi^{-1}})}.$$

Since $\overline{\xi^{-1}} = \frac{q}{p}e^{i\delta}$ we may let tend $\delta \to \frac{\pi}{2}$ by Theorem 1. Hence

$$R^2(s) = T_0\left(s, i\frac{p}{q}\right) + \overline{T_0\left(1-\overline{s}, i\frac{q}{p}\right)} + H\left(s, i\frac{p}{q}\right),$$

from which our assertion is obvious.

This result shows that the study of $\zeta^2(s)$ is reduced to that of $T(s,\frac{p}{q})$ for positive, coprime integers p,q. Obviously, $T(s,\frac{p}{q})$ is an integral function of s if p and q are fixed. Our final goal will be to derive an analogue of the Riemann-Siegel integral formula for $T(s,\frac{p}{q})$. As it turns out, the formulas to be established depend on the properties of certain integral transforms of $\psi(x)$, which we are going to investigate next.

2. Integral Transforms Involving $\psi(x)$

Let p,q be integers, $q \neq 0$, and consider for $z \in \mathbf{C}$ with $\mathrm{Re}(z) > 0$ the integral

$$\mathcal{K}(p,q,z) = \int_{i\frac{p}{q}}^{i\frac{p}{q}+\infty} K_0(2\pi xz)x\psi(x)\mathrm{d}x. \tag{2.1}$$

Since $K_0(2\pi xz) = O\big(|(xz)^{-\frac{1}{2}}e^{-2\pi xz}|\big)$ and $\psi(x) = O(e^{-2\pi\mathrm{Re}(x)})$ for $\mathrm{Re}(x) \to \infty$ by (1.2), it is seen that the integral converges absolutely at its upper bound since $\mathrm{Re}(z) > 0$. In the vicinity of $i\frac{p}{q}$, Theorems 1 and 2 imply $\psi(x+i\frac{p}{q}) = O(x^{-\frac{1}{2}}|\log x|)$ for $x \to 0$, while $K_0\big(2\pi(i\frac{p}{q}+x)z\big)$ is regular (if $p \neq 0$) or has a logarithmic singularity (if $p = 0$). This shows that $\mathcal{K}(p,q,\cdot)$ defines a function holomorphic in the right half plane $\mathrm{Re}(z) > 0$.

This function is fundamental in our subsequent analysis and in the present section we proceed to derive its basic properties.

Lemma 5: *Let p,q be integers, $p \neq 0$, $q \neq 0$. Then for non integral $z \in \mathbf{C}$*

$$\mathcal{K}(p,q,z) = \frac{2ip}{\pi q}\sum_{n=1}^{\infty}\frac{d(n)}{n^2-z^2}\big[zK_0(2\pi in\tfrac{p}{q})K_0'(2\pi iz\tfrac{p}{q}) - nK_0'(2\pi in\tfrac{p}{q})K_0(2\pi iz\tfrac{p}{q})\big].$$

The series converges absolutely and uniformly for z contained in any compact subset of the complex plane excluding the integers.

Proof: Let $\mathrm{Re}(z) > 0$. In the above definition of $\mathcal{K}(p,q,z)$ we insert the series (1.2) for $\psi(x)$ and invert the the order of integration and summation. This is permitted, for instance, by Lebesgue's theorem on dominated convergence. Hence

$$\mathcal{K}(p,q,z) = \pi^{-2}\sum_{n=1}^{\infty} d(n)n^{-2}\int_{2\pi inp/q}^{2\pi inp/q+\infty} uK_0(u)K_0(\tfrac{z}{n}u)\mathrm{d}u.$$

Now observe that integrals of the type

$$\int uK_0(u)K_0(\alpha u)\mathrm{d}u$$

can be explicitly computed. To show this, consider the function $f(u) = K_0'(u)K_0(\alpha u) - \alpha K_0(u)K_0'(\alpha u)$, where α is a complex number. Using the differential equation $uK_0''(u) = uK_0(u) - K_0'(u)$, we have

$$\big[uf(u)\big]' = uf'(u) + f(u) = (1-\alpha^2)uK_0(u)K_0(\alpha u).$$

Thus $\int uK_0(u)K_0(\alpha u)\mathrm{d}u = (1-\alpha^2)^{-1}uf(u)$. With $\alpha = \frac{z}{n}$ and $\lambda := 2\pi i\frac{p}{q}$, we get

$$\int_{n\lambda}^{n\lambda+\infty} uK_0(u)K_0(\tfrac{z}{n}u)\mathrm{d}u = \lambda\frac{n^2}{n^2-z^2}\big[zK_0(\lambda n)K_0'(\lambda z) - nK_0'(\lambda n)K_0(\lambda z)\big].$$

From this formula the assertions follow at once since $K_0(\lambda n) = O(n^{-\frac{1}{2}})$, $K_0'(\lambda n) = O(n^{-\frac{1}{2}})$.

Since the Bessel function $K_0(u)$ has a logarithmic singularity at $u = 0$, it is convenient to introduce a cut along the positive imaginary axis. Then $-\frac{3\pi}{2} < \arg(z) < \frac{\pi}{2}$ in the cut plane, or, equivalently, $-\pi < \arg(iz) < \pi$. The main analytic properties of $\mathcal{K}(p,q,z)$ follow directly from the previous lemma. We have first

Theorem 3: *Let p,q be positive integers. Then $\mathcal{K}(p,q,\cdot)$ extends to a meromorphic function in the plane cut from 0 to $i\infty$. It has simple poles at the negative integers $z = -n = e^{-\pi i}n$ with residue being equal to $-\frac{d(n)}{4\pi i n}$, and is regular elsewhere.*

Proof: We use Lemma 5. Write $x = 2\pi\frac{p}{q} > 0$ and

$$f_n(z) = zK_0(inx)K_0'(izx) - nK_0'(inx)K_0(izx),$$

so that

$$\mathcal{K}(p,q,z) = \frac{2ip}{\pi q}\sum_{n=1}^{\infty}\frac{d(n)}{n^2-z^2}f_n(z).$$

Since $f_n(z)$ is analytic in the cut plane, except for possible poles at $z = \pm n$, the first assertion follows from absolute and uniform convergence of the series in compact subsets of the plane, excluding the integers. Noting that $f_n(n) = 0$, it follows moreover that $\mathcal{K}(p,q,z)$ is regular at $z = n$. Its value is easily computed to be

$$\mathcal{K}(p,q,n) = \frac{\lambda}{\pi^2}\sum_{m\neq n}\frac{d(m)}{m^2-n^2}\big[nK_0(\lambda m)K_0'(\lambda n) - mK_0'(\lambda m)K_0(\lambda n)\big] - \frac{\lambda}{2\pi^2 n},$$

where $\lambda = 2\pi i\frac{p}{q}$. This proves the assertions on the analytical character of $\mathcal{K}(p,q,z)$, and it remains to compute the residue at $z = -n = e^{-\pi i}n$. The task is facilitated by introducing the Hankel functions $H_\nu^{(a)}$ with $\nu \in \{0,1\}$, $a \in \{1,2\}$. Let $x > 0$. Then, as is well known ([5, p.109], [10, p. 78])

$$K_\nu(ix) = -\frac{\pi i}{2}e^{-\frac{\pi i\nu}{2}}H_\nu^{(2)}(x), \quad K_\nu(-ix) = \frac{\pi i}{2}e^{\frac{\pi i\nu}{2}}H_\nu^{(1)}(x). \tag{2.2}$$

Using also $K_0' = -K_1$, we can write with $x = 2\pi\frac{p}{q}$

$$\begin{aligned} f_n(e^{-\pi i}n) &= nK_0(inx)K_1(-inx) + nK_1(inx)K_0(-inx) \\ &= \frac{\pi^2 i}{4}n\big[H_0^{(2)}(nx)H_1^{(1)}(nx) - H_0^{(1)}(nx)H_1^{(2)}(nx)\big]. \end{aligned}$$

Since $\frac{\mathrm{d}}{\mathrm{d}z}H_0^{(a)} = -H_1^{(a)}$, it is seen that the bracketed term is nothing but the Wronskian of the pair $H_0^{(1)}, H_0^{(2)}$ at nx, which equals $-\frac{4i}{\pi nx}$. Thus $f_n(-n) = \frac{q}{2p}$, and this concludes the proof of Theorem 3.

We next show how to continue $\mathcal{K}(p,q,z)$ across the cut from 0 to $i\infty$. To this end we use the formulae [10, p.80]

$$K_\nu(ze^{\pi im}) = (-1)^{m\nu}\big[K_\nu(z) - (-1)^\nu \pi im I_\nu(z)\big], \tag{2.3}$$

valid for all integers ν and m. Hence

$$f_n(ze^{\pi im}) = -(-1)^m zK_0(\lambda n)K_1(\lambda ze^{\pi im}) + nK_1(\lambda n)K_0(\lambda ze^{\pi im}) = f_n(z) - \pi im g_n(z),$$

where

$$g_n(z) = zK_0(\lambda n)I_1(\lambda z) + nK_1(\lambda n)I_0(\lambda z) \tag{2.4}$$

and $\lambda = 2\pi i\frac{p}{q}$. We have therefore proved part of

Theorem 4: *Let p, q be positive integers, m be any integer, and z complex but not an integer. Then $\mathcal{K}(p,q,ze^{\pi i m}) = \mathcal{K}(p,q,z) + m\mathcal{G}(p,q,z)$ with*

$$\mathcal{G}(p,q,z) = \frac{2p}{q}\sum_{n=1}^{\infty}\frac{d(n)}{n^2-z^2}\big[zK_0(\lambda n)I_1(\lambda z) + nK_1(\lambda n)I_0(\lambda z)\big], \quad \lambda = 2\pi i\frac{p}{q}.$$

The function $\mathcal{G}(p,q,\cdot)$ is an even meromorphic function in the entire plane. Its only singularities are simple poles at $z = \pm n$ (n positive integer) with residue being equal to $\mp\frac{d(n)}{2\pi i n}$.

Proof: The equations for $\mathcal{K}(p,q,ze^{\pi i m})$ and $\mathcal{G}(p,q,z)$ follow immediately from the formula for $f_n(ze^{\pi i m})$ derived above. Since $K_\nu(2\pi i n\frac{p}{q}) = O(n^{-\frac{1}{2}})$ for $n \to \infty$ and I_ν is an entire function, the analytic character of $\mathcal{G}(p,q,\cdot)$ is also obvious. Its evenness follows from $I_\nu(-z) = (-1)^\nu I_\nu(z)$, provided ν is an integer. To compute the residues, observe that

$$\begin{aligned} g_n(n) &= nK_0(\lambda n)I_1(\lambda n) + nK_1(\lambda n)I_0(\lambda n) = -n\big[I_0(\lambda n)K_0'(\lambda n) - I_0'(\lambda n)K_0(\lambda n)\big] \\ &= -n\left(-\frac{1}{\lambda n}\right) = \frac{1}{\lambda} = \frac{q}{2\pi i p}, \end{aligned}$$

and this completes the proof of the theorem.

Another method to derive the formula of Theorem 4 is to use the definition

$$\mathcal{K}(p,q,z) = \int_{i\frac{p}{q}}^{\infty + i\frac{p}{q}} K_0(2\pi x z)x\psi(x)\mathrm{d}x.$$

Assume temporarily $-1 < \mathrm{Re}(z) < 1$. Then by (2.3)

$$\begin{aligned} \mathcal{K}(p,q,ze^{\pi i m}) &= \int_{i\frac{p}{q}}^{\infty + i\frac{p}{q}} \big[K_0(2\pi x z) - \pi i m I_0(2\pi x z)\big]x\psi(x)\mathrm{d}x \\ &= \mathcal{K}(p,q,z) - \pi i m \int_{i\frac{p}{q}}^{\infty + i\frac{p}{q}} I_0(2\pi x z)x\psi(x)\mathrm{d}x. \end{aligned}$$

The last integral converges absolutely in view of $I_0(w) = O(e^{|\mathrm{Re}(w)|})$ and $\psi(x) = O(e^{-2\pi x})$. Now

$$\int_{i\frac{p}{q}}^{\infty + i\frac{p}{q}} I_0(2\pi x z)x\psi(x)\mathrm{d}x = \frac{1}{\pi^2}\sum_{n=1}^{\infty} d(n)n^{-2}\int_{2\pi i n p/q}^{\infty + 2\pi i n p/q} uK_0(u)I_0(\tfrac{z}{n}u)\mathrm{d}u.$$

These integrals can be computed in much the same way as those above, the result being

$$\int uK_0(u)I_0(\alpha u)\mathrm{d}u = (1-\alpha^2)^{-1}u\big[K_0'(u)I_0(\alpha u) - \alpha K_0(u)I_0'(\alpha u)\big].$$

Hence (with $\lambda = 2\pi i p/q$)

$$\int_{i\frac{p}{q}}^{\infty + i\frac{p}{q}} I_0(2\pi x z)x\psi(x)\mathrm{d}x = \frac{2ip}{\pi q}\sum_{n=1}^{\infty}\frac{d(n)}{n^2-z^2}\big[zK_0(\lambda n)I_0'(\lambda z) - nK_0'(\lambda n)I_0(\lambda z)\big].$$

Inserting this into the above representation for $\mathcal{K}(p,q,ze^{\pi i m})$, we get $\mathcal{K}(p,q,ze^{\pi i m}) = \mathcal{K}(p,q,z) + m\mathcal{G}(p,q,z)$, where

$$\mathcal{G}(p,q,z) = -\pi i \int_{i\frac{p}{q}}^{\infty + i\frac{p}{q}} I_0(2\pi x z) x \psi(x) \mathrm{d}x \tag{2.5}$$

$$= \frac{2p}{q} \sum_{n=1}^{\infty} \frac{d(n)}{n^2 - z^2} \big[z K_0(\lambda n) I_0'(\lambda z) - n K_0'(\lambda n) I_0(\lambda z) \big], \tag{2.6}$$

which coincides with the result of Theorem 4. In the last formula the restriction $-1 < \mathrm{Re}(z) < 1$ can be removed by absolute convergence if z is not equal to any integer.

In later applications it will prove convenient to introduce two further functions connected with $\mathcal{G}(p,q,z)$. For this purpose we use the relations [10, p.74, 77] $I_0(z) = J_0(z/i) = \frac{1}{2}\big[H_0^{(1)}(z/i) + H_0^{(2)}(z/i)\big]$. Then with

$$\mathcal{G}^{(a)}(p,q,z) = -\frac{\pi i}{2} \int_{i\frac{p}{q}}^{i\frac{p}{q}+\infty} H_0^{(a)}(2\pi x z/i) x \psi(x) \mathrm{d}x, \quad a \in \{1,2\}, \tag{2.7}$$

we clearly have the decomposition

$$\mathcal{G}(p,q,z) = -\frac{\pi i}{2} \big[\mathcal{G}^{(1)}(p,q,z) + \mathcal{G}^{(2)}(p,q,z) \big]. \tag{2.8}$$

Explicit formulas for $\mathcal{G}^{(a)}$ can be obtained as usual. Inserting the definition of $\psi(x)$ yields

$$\mathcal{G}^{(a)}(p,q,z) = \frac{1}{\pi^2} \sum_{n=1}^{\infty} \frac{d(n)}{n^2} \int_{2\pi i n p/q}^{2\pi i n p/q + \infty} u K_0(u) H_0^{(a)}\left(\frac{zu}{in}\right) \mathrm{d}u.$$

From the differential equation $H_0^{(a)\prime\prime}(z) + z^{-1} H_0^{(a)\prime}(z) + H_0^{(a)}(z) = 0$ we get

$$\int u K_0(u) H_0^{(a)}(\alpha u) \mathrm{d}u = (1+\alpha^2)^{-1} u \big[K_0'(u) H_0^{(a)}(\alpha u) - \alpha K_0(u) H_0^{(a)\prime}(\alpha u) \big].$$

Therefore with $\mu = 2\pi p/q$

$$\int_{in\mu}^{in\mu+\infty} u K_0(u) H_0^{(a)}\left(\frac{zu}{in}\right) \mathrm{d}u = \frac{\pi i \mu n^2}{2(n^2 - z^2)} \big[z H_0^{(2)}(\mu n) H_1^{(a)}(\mu z) - n H_1^{(2)}(\mu n) H_0^{(a)}(\mu z) \big],$$

where again the relations (2.2) and $K_0' = -K_1$, $H_0^{(a)\prime} = -H_1^{(a)}$ have been employed. This leads to the following representation:

$$\mathcal{G}^{(a)}(p,q,z) = \frac{ip}{q} \sum_{n=1}^{\infty} \frac{d(n)}{n^2 - z^2} \big[z H_0^{(2)}(\mu n) H_1^{(a)}(\mu z) - n H_1^{(2)}(\mu n) H_0^{(a)}(\mu z) \big], \quad \mu = 2\pi \frac{p}{q}. \tag{2.9}$$

From $H_0^{(a)}(\mu n) = O(n^{-\frac{1}{2}})$ for $n \to \infty$, it is easily deduced that both functions are regular in the complex plane cut along the negative real axis, except for possible poles at $z = n$ or $z = e^{-\pi i} n$.

In order to determine the behaviour in these points we define

$$f_n^{(a)}(z) = z H_0^{(2)}(\mu n) H_1^{(a)}(\mu z) - n H_1^{(2)}(\mu n) H_0^{(a)}(\mu z).$$

Then

$$f_n^{(1)}(n) = n \big[H_0^{(2)}(\mu n) H_1^{(1)}(\mu n) - H_1^{(2)}(\mu n) H_0^{(1)}(\mu n) \big]$$
$$= n \big[H_0^{(1)}(\mu n) H_0^{(2)\prime}(\mu n) - H_0^{(1)\prime}(\mu n) H_0^{(2)}(\mu n) \big] = -\frac{2iq}{\pi^2 p},$$

on using the Wronski determinant for $H_0^{(1)}, H_0^{(2)}$ ([5, p. 113], [10, p.76]). Concerning $z = e^{-\pi i}n$ we have [10, p.75]

$$H_0^{(1)}(e^{-\pi i}z) = 2H_0^{(1)}(z) + H_0^{(2)}(z), \quad H_0^{(2)}(e^{-\pi i}z) = -H_0^{(1)}(z),$$

and

$$H_1^{(1)}(e^{-\pi i}z) = -2H_1^{(1)}(z) - H_1^{(2)}(z), \quad H_1^{(2)}(e^{-\pi i}z) = H_1^{(1)}(z).$$

Consequently,

$$f_n^{(1)}(e^{-\pi i}n) = -n\big[-2H_0^{(2)}(\mu n)H_1^{(1)}(\mu n) + 2H_1^{(2)}(\mu n)H_0^{(1)}(\mu n)\big] = -\frac{4iq}{\pi^2 p}.$$

Turning to $f_n^{(2)}$ we clearly have $f_n^{(2)}(n) = 0$. Moreover,

$$f_n^{(2)}(e^{-\pi i}n) = -n\big[H_0^{(2)}(\mu n)H_1^{(1)}(\mu n) - H_1^{(2)}(\mu n)H_0^{(1)}(\mu n)\big] = \frac{2iq}{\pi^2 p}.$$

Collecting all these results we have

Theorem 5: *The functions $\mathcal{G}^{(a)}(p,q,\cdot)$ as defined in (2.7) are meromorphic in the plane cut from 0 to $-\infty$. $\mathcal{G}^{(1)}$ has a simple pole at $z = n$ with residue $-\frac{d(n)}{\pi^2 n}$, and a simple pole at $z = e^{-\pi i}n$ with residue $\frac{2d(n)}{\pi^2 n}$. The function $\mathcal{G}^{(2)}$ is regular for $-\pi < \arg(z) < \pi$ and has a simple pole at $z = e^{-\pi i}n$ with residue $-\frac{d(n)}{\pi^2 n}$.*

For many purposes it is necessary to have asymptotic estimates about the growth of the fundamental functions $\mathcal{K}(p,q,z)$ and $\mathcal{G}^{(a)}(p,q,z)$ for $z \to \infty$. The most basic one is given by

Theorem 6: *Let p, q be positive integers, and δ, A be positive real numbers such that $\frac{p}{q} \geq A$. Let z be complex, $r = |z| \geq 2$, $M = \min\{|z-n|; n \in \mathbf{Z}\}$ and assume $M \neq 0$. Then $\mathcal{K}(p,q,z) = e^{-2\pi izp/q}\mathcal{K}_0(p,q,z)$, where $\mathcal{K}_0(p,q,\cdot)$ is meromorphic in the plane cut from 0 to $i\infty$ and satisfies*

$$\mathcal{K}_0(p,q,z) \ll (1+M^{-1})r^{-\frac{1}{2}}\log r, \quad -2\pi + \delta \leq \arg(z) \leq \pi - \delta,$$

uniformly in p, q, z. Similarly,

$$\mathcal{G}^{(1)}(p,q,z) = e^{2\pi izp/q}\mathcal{G}_0^{(1)}(p,q,z), \quad \mathcal{G}^{(2)}(p,q,z) = e^{-2\pi izp/q}\mathcal{G}_0^{(2)}(p,q,z),$$

where

$$\mathcal{G}_0^{(1)}(p,q,z) \ll (1+M^{-1})r^{-\frac{1}{2}}\log r, \quad -\pi + \delta \leq \arg(z) \leq 2\pi - \delta,$$
$$\mathcal{G}_0^{(2)}(p,q,z) \ll (1+M^{-1})r^{-\frac{1}{2}}\log r, \quad -2\pi + \delta \leq \arg(z) \leq \pi - \delta,$$

uniformly in p, q, z.

Proof: Consider first $\mathcal{K}(p,q,z)$. Write $K_\nu(z) = (\frac{\pi}{2z})^{\frac{1}{2}}e^{-z}K_\nu^*(z)$. Then K_ν^* is holomorphic in the plane cut from 0 to $-\infty$. Moreover, if $|z| \geq 1$, $|\arg(z)| \leq \frac{3\pi}{2} - \delta$, then, by the asymptotic expansion for the modified Bessel function ([8, p. 250], [10, p. 202]), K_ν^* is bounded. This remains true if we assume $|z| \geq A$ for some positive constant A. This follows easily from $K_0(z) = O(\log z)$, $K_\nu(z) = O(z^{-\nu})$ $(\nu \geq 1)$ as $z \to 0$. Hence we can write

$$K_\nu\left(2\pi iz\frac{p}{q}\right) = \left(4iz\frac{p}{q}\right)^{-\frac{1}{2}} e^{-2\pi izp/q}K_\nu^*\left(2\pi iz\frac{p}{q}\right), \quad -2\pi + \delta \leq \arg(z) \leq \pi - \delta,\ 2\pi|z|\frac{p}{q} \gg 1.$$

With the abbreviation $\lambda = 2\pi i\frac{p}{q}$, Lemma 5 gives

$$\mathcal{K}(p,q,z) = -\frac{e^{\frac{\pi i}{4}}}{\pi}\left(\frac{p}{q}\right)^{\frac{1}{2}} z^{-\frac{1}{2}}e^{-2\pi izp/q}\sum_{n=1}^{\infty}\frac{d(n)}{n^2 - z^2}\big[zK_0(\lambda n)K_1^*(\lambda z) + nK_0'(\lambda n)K_0^*(\lambda z)\big]. \qquad (2.10)$$

Now we use $K_\nu(\lambda n) = O\big((\lambda n)^{-\frac12}\big)$. By the asymptotic formula above, this is true for $|\lambda n| \ge 1$ and, more generally, for all $n \ge 1$, since $|\lambda n| \ge |\lambda| \ge 2\pi A > 0$. Thus with $\frac{1}{n^2-z^2} = \frac{1}{2z}\big(\frac{1}{n-z} - \frac{1}{n+z}\big)$ we get

$$\sum_{n=1}^{\infty} \frac{d(n)}{n^2 - z^2} z K_0(\lambda n) K_1^*(\lambda z) \ll \left(\frac{p}{q}\right)^{-\frac12} \sum_{n=1}^{\infty} d(n) n^{-\frac12} \big(|n-z|^{-1} + |n+z|^{-1}\big). \tag{2.11}$$

Similarly, with $\frac{1}{n^2-z^2} = \frac{1}{2n}\big(\frac{1}{n-z} + \frac{1}{n+z}\big)$

$$\sum_{n=1}^{\infty} \frac{d(n)}{n^2 - z^2} n K_0'(\lambda n) K_0^*(\lambda z) \ll \left(\frac{p}{q}\right)^{-\frac12} \sum_{n=1}^{\infty} d(n) n^{-\frac12} \big(|n-z|^{-1} + |n+z|^{-1}\big). \tag{2.12}$$

We are therefore reduced to estimate the last infinite series. It suffices clearly to assume $\mathrm{Re}(z) \ge 0$. Then $|n+z| \ge n$ which yields $\sum d(n) n^{-\frac12} |n+z| \le \zeta^2(\frac32) = O(1)$. It remains to consider $S(z) = \sum d(n) n^{-\frac12} |n-z|^{-1}$. With $r = |z|$ we split the summation into three parts.

For $n \le r - \sqrt{r}$ we have $|n - z| \ge r - n \ge \sqrt{r}$. Thus

$$\sum_{n \le r - \sqrt{r}} d(n) n^{-\frac12} |n-z|^{-1} \ll r^{-\frac12} \sum_{n \le r - \sqrt{r}} d(n) n^{-\frac12} \ll \log r.$$

Now consider the interval $r - \sqrt{r} < n \le r + \sqrt{r}$. Since $|n - z| \ge M$ always, we get

$$\sum_{r-\sqrt{r} < n \le r + \sqrt{r}} d(n) n^{-\frac12} |n-z|^{-1} \le M^{-1} r^{-\frac12} \sum_{r-\sqrt{r} < n \le r + \sqrt{r}} d(n) \ll M^{-1} \log r.$$

Finally, consider those n satisfying $n > r + \sqrt{r}$. Note first that the inequality implies $\frac{r}{n} < (1 + r^{-\frac12})^{-1}$ and thus

$$|n - z| \ge n - r = n(1 - \tfrac{r}{n}) > n\big(1 + r^{\frac12}\big)^{-1} \ge \frac{n}{2\sqrt{r}}.$$

Consequently,

$$\sum_{n > r + \sqrt{r}} d(n) n^{-\frac12} |n-z|^{-1} \ll r^{\frac12} \sum_{n > r + \sqrt{r}} d(n) n^{-\frac32} \ll \log r.$$

Thus we have shown $S(z) \ll \log r + M^{-1} \log r$, provided $r \ge 2$. Inserting (2.11) and (2.12) into (2.10) yields the desired assertion.

Similar reasoning applies to $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$ using the explicit formula (2.9). This proves the theorem.

For certain purposes [2] it is convenient to use another representation of the the functions $\mathcal{G}^{(a)}(p, q, \cdot)$, which is essentially a Laplace transform. To this end define

$$\psi_\nu(x) = \sum_{n=1}^{\infty} d(n) H_\nu^{(2)}(\mu n) e^{-\mu n x}, \quad \mu = 2\pi \frac{p}{q}, \ \mathrm{Re}(x) > 0, \tag{2.13}$$

and

$$L_\nu(z) = \mu \int_0^\infty e^{\mu z x} \psi_\nu(x) \mathrm{d}x, \quad \mathrm{Re}(z) < 1. \tag{2.14}$$

It is easily seen that $\psi_\nu(x) = O(x^{-\frac12} \log x)$ for $x \to 0$ and $\psi_\nu(x) = O(e^{-\mu x})$ for $x \to +\infty$. Hence the integral converges absolutely and uniformly for $\mathrm{Re}(z) \le 1 - \varepsilon$, where $\varepsilon > 0$ is fixed. This implies that L_ν is holomorphic in the left half plane $\mathrm{Re}(z) < 1$. Its analytic continuation is found by inserting the series (2.13) into (2.14) and integrating term by term, the result being

$$L_\nu(z) = \sum_{n=1}^{\infty} d(n) H_\nu^{(2)}(\mu n) \frac{1}{n - z}. \tag{2.15}$$

From this explicit representation we conclude that L_ν extends to a meromorphic function. The only singularities are simple poles at the positive integers $z = n$ with residue $-d(n)H_\nu^{(2)}(\mu n)$. We then have

Theorem 7: *Let p, q be positive integers and define ψ_ν and L_ν as in (2.13) and (2.14), respectively. Then for $a \in \{1, 2\}$*

$$\mathcal{G}^{(a)}(p,q,z) = \frac{ip}{2q} H_1^{(a)}(\mu z)\big[L_0(z) - L_0(-z)\big] - \frac{ip}{2q} H_0^{(a)}(\mu z)\big[L_1(z) - L_1(-z)\big],$$

where $\mu = 2\pi \frac{p}{q}$.

Proof: Write (2.9) in the form

$$\mathcal{G}^{(a)}(p,q,z) = \frac{ip}{q} \sum_{n=1}^{\infty} \frac{d(n)}{n^2 - z^2} z a_n H_1^{(a)}(\mu z) - \frac{ip}{q} \sum_{n=1}^{\infty} \frac{d(n)}{n^2 - z^2} n b_n H_0^{(a)}(\mu z),$$

with $a_n = H_0^{(2)}(\mu n)$, $b_n = H_1^{(2)}(\mu n)$. Note that $a_n = O(n^{-\frac{1}{2}})$ and $b_n = O(n^{-\frac{1}{2}})$, provided μ is fixed. Using $\frac{1}{n^2-z^2} = \frac{1}{2n}(\frac{1}{n-z} + \frac{1}{n+z}) = \frac{1}{2z}(\frac{1}{n-z} - \frac{1}{n+z})$, we obtain

$$\mathcal{G}^{(a)}(p,q,z) = \frac{ip}{q} H_1^{(a)}(\mu z) \sum_{n=1}^{\infty} d(n) a_n (\tfrac{1}{n-z} - \tfrac{1}{n+z}) - \frac{ip}{q} H_0^{(a)}(\mu z) \sum_{n=1}^{\infty} d(n) b_n (\tfrac{1}{n-z} + \tfrac{1}{n+z}).$$

Assuming $-1 < \mathrm{Re}(z) < 1$, we can write

$$\frac{1}{n-z} = \int_0^\infty e^{-u(n-z)} \mathrm{d}u, \qquad \frac{1}{n+z} = \int_0^\infty e^{-u(n+z)} \mathrm{d}u.$$

Hence

$$\begin{aligned}\mathcal{G}^{(a)}(p,q,z) = {} & \frac{ip}{2q} H_1^{(a)}(\mu z) \sum_{n=1}^{\infty} d(n) a_n \left(\int_0^\infty e^{-un+uz} \mathrm{d}u - \int_0^\infty e^{-un-uz} \mathrm{d}u \right) \\ & - \frac{ip}{2q} H_0^{(a)}(\mu z) \sum_{n=1}^{\infty} d(n) b_n \left(\int_0^\infty e^{-un+uz} \mathrm{d}u + \int_0^\infty e^{-un-uz} \mathrm{d}u \right).\end{aligned}$$

Interchanging the order of integration and summation, which is permitted by absolute convergence, immediately yields the claim. This proves Theorem 7.

3. The Riemann-Siegel Integral Formula

From our previous investigations we can now derive some new integral representations for $\zeta^2(s)$. Thus assume $\sigma < 2$, $0 < \varphi < \pi$, and let p, q be positive integers. Using the reflection formula for the gamma function we obtain

$$\Gamma\left(\frac{s}{2}\right)^{-2} = \frac{1 - \cos \pi s}{2\pi^2} \Gamma\left(\frac{2-s}{2}\right)^2 = 2^{s-1} \pi^{-2} (1 - \cos \pi s) \int_0^\infty K_0(z) z^{1-s} \mathrm{d}z.$$

Let $\mathrm{Re}(\alpha) > 0$. Then substitute $z = \alpha u$ and turn the line of integration about the origin to get

$$\Gamma\left(\frac{s}{2}\right)^{-2} = 2^{s-1} \pi^{-2} (1 - \cos \pi s) \alpha^{2-s} \int_0^{\infty e^{-i\varphi}} K_0(\alpha u) u^{1-s} \mathrm{d}u,$$

provided $|\arg(\alpha) - \varphi| < \frac{\pi}{2}$. In particular, let $\alpha = 2\pi x$, where $\mathrm{Re}(x) \geq 0$ and $\mathrm{Im}(x) = \frac{p}{q}$. Consequently, if $0 \leq \varphi \leq \frac{\pi}{2}$,

$$\pi^s \Gamma\left(\frac{s}{2}\right)^{-2} = 2(1 - \cos \pi s) x^{2-s} \int_0^{\infty e^{-i\varphi}} K_0(2\pi x u) u^{1-s} \mathrm{d}u.$$

Multiplying by $\psi(x)x^{s-1}$ and integrating from $i\frac{p}{q}$ to $i\frac{p}{q}+\infty$ yields

$$\begin{aligned}
T(s) &= \pi^s \Gamma\left(\frac{s}{2}\right)^{-2} \int_{i\frac{p}{q}}^{i\frac{p}{q}+\infty} \psi(x)x^{s-1}\mathrm{d}x \\
&= 2(1-\cos\pi s)\int_{i\frac{p}{q}}^{i\frac{p}{q}+\infty} x\psi(x)\int_0^{\infty e^{-i\varphi}} K_0(2\pi x u)u^{1-s}\mathrm{d}u\mathrm{d}x \\
&= 2(1-\cos\pi s)\int_0^{\infty e^{-i\varphi}} u^{1-s}\int_{i\frac{p}{q}}^{i\frac{p}{q}+\infty} xK_0(2\pi xu)\psi(x)\mathrm{d}x\mathrm{d}u,
\end{aligned}$$

where the interchange of the order of integration is permitted by absolute convergence of the double integral. Hence

$$T(s) = 2(1-\cos\pi s)\int_0^{\infty e^{-i\varphi}} \mathcal{K}(p,q,u)u^{1-s}\mathrm{d}u. \tag{3.1}$$

In this equation even $\varphi < \pi$ is allowed, since $\mathcal{K}(p,q,u) = O(e^{-2\pi \mathrm{Re}(iu)p/q})$ for $u \to \infty$ (Theorem 6). Together with Theorem 2 this constitutes our first analogue of the Riemann-Siegel integral formula for $\zeta^2(s)$.

It is also possible to obtain formulas involving the functions $\mathcal{G}^{(a)}$ introduced in Section 2. It will be seen that these representations are even more elegant. First assume $\frac{3}{2} < \sigma < 2$, and let L denote the path consisting of the straight line segments from 0 to $-1-i$ and from $-1-i$ to $-i-\infty$. By Theorem 6 and (3.1) above

$$T(s) = 2(1-\cos\pi s)\int_L \mathcal{K}(p,q,u)u^{1-s}\mathrm{d}u.$$

If we set $z = e^{\pi i}w$, we obtain

$$\begin{aligned}
T(s) &= 2(1-\cos\pi s)e^{\pi i s}\int_{e^{\pi i}L} \mathcal{K}(p,q,e^{-\pi i}z)z^{1-s}\mathrm{d}z \\
&= 2(1-\cos\pi s)e^{\pi i s}\int_{e^{\pi i}L} \big[\mathcal{K}(p,q,z) - \mathcal{G}(p,q,z)\big]z^{1-s}\mathrm{d}z.
\end{aligned}$$

Since $\mathcal{K}(p,q,\cdot)$ is regular for $-\pi < \arg(z) < \frac{\pi}{2}$ and decays sufficiently fast for $|z| \to \infty$ (Theorem 6), the integral involving $\mathcal{K}(p,q,\cdot)$ can be turned around the origin, so that

$$\int_{e^{\pi i}L} \mathcal{K}(p,q,z)z^{1-s}\mathrm{d}z = \int_L \mathcal{K}(p,q,z)z^{1-s}\mathrm{d}z.$$

This gives

$$\begin{aligned}
T(s) &= 2(1-\cos\pi s)e^{\pi i s}\left\{\int_L \mathcal{K}(p,q,z)z^{1-s}\mathrm{d}z - \int_{e^{\pi i}L} \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z\right\} \\
&= e^{\pi i s}T(s) - 2(1-\cos\pi s)e^{\pi i s}\int_{e^{\pi i}L} \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z,
\end{aligned}$$

or, equivalently,

$$(e^{\pi i s} - 1)T(s) = 2(1-\cos\pi s)\int_L \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z. \tag{3.2}$$

Now consider the integral

$$I = \int_\Lambda \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z,$$

where Λ denotes the path from $-\infty - i$ to $e^{-\frac{3\pi i}{4}}\delta$ $(0 < \delta < 1)$, then along the circle of radius δ around the origin from $e^{-\frac{3\pi i}{4}}\delta$ to $e^{\frac{\pi i}{2}}\delta$, and finally from $e^{\frac{\pi i}{2}}\delta$ to $\infty + i$. By assumption $\frac{3}{2} < \sigma < 2$. This implies that the integral converges absolutely for $\delta \to 0$, as well as at infinity, using, in addition, the estimate of Theorem 6. Thus we may let tend δ to 0, leading to

$$I = \left(\int_{-\infty-i}^{0} + \int_{0}^{\infty+i}\right) \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z = -\int_L \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z + \int_{e^{\pi i}L} \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z$$
$$= (e^{-\pi i s} - 1)\int_L \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z,$$

since $\mathcal{G}(p,q,-z) = \mathcal{G}(p,q,z)$. Inserting this expression into (3.2) yields

$$(e^{\pi i s} - 1)T(s) = 2(1-\cos\pi s)(e^{-\pi i s} - 1)^{-1}I,$$

i.e.

$$T(s) = \int_\Lambda \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z = (1-e^{\pi i s})\int_0^{i+\infty} \mathcal{G}(p,q,z)z^{1-s}\mathrm{d}z. \tag{3.3}$$

To ensure absolute convergence, we had to assume $\frac{3}{2} < \sigma < 2$, but it might well be that these formulas continue to hold for a wider range of σ. A more detailed investigation of the properties of $\mathcal{G}(p,q,z)$ will perhaps reveal this property. It is, however, possible to employ another, more elementary, method. In fact, using the decomposition (2.8) we get

$$T(s) = \frac{\pi}{2i}(1-e^{\pi i s})\int_0^{i+\infty}\left[\mathcal{G}^{(1)}(p,q,z) + \mathcal{G}^{(2)}(p,q,z)\right]z^{1-s}\mathrm{d}z.$$

By Theorem 6 we may modify the path of integration in such a manner that $\mathrm{Im}(z) \to +\infty$ for $\mathcal{G}^{(1)}$ and $\mathrm{Im}(z) \to -\infty$ for $\mathcal{G}^{(2)}$. Thus for any φ with $0 \le \varphi < \frac{\pi}{2}$

$$T(s) = \frac{\pi}{2i}(1-e^{\pi i s})\left\{\int_0^{\infty e^{i\varphi}} \mathcal{G}^{(1)}(p,q,z)z^{1-s}\mathrm{d}z + \int_0^{\infty e^{-i\varphi}} \mathcal{G}^{(2)}(p,q,z)z^{1-s}\mathrm{d}z\right\}. \tag{3.4}$$

Here it should be remembered that $\mathcal{G}^{(1)}(p,q,\cdot)$ is holomorphic in the upper half plane, and $\mathcal{G}^{(2)}(p,q,\cdot)$ is holomorphic in the right half plane $\mathrm{Re}(z) > 0$ (Theorem 5). Thus we have obtained the desired analytic continuation, as the integrals in (3.3) are absolutely convergent for any $\sigma < 2$. Since $\zeta^2(s)$ is given in terms of $T(s)$ and an elementary function (Theorem 2), formulas (3.1), (3.3), and (3.4) can be considered as the desired analogue of the Riemann-Siegel formula.

It is the last equation (3.4) that may serve as a starting point for the derivation of the asymptotic expansion of $\zeta^2(s)$. To illustrate this point and to show the utility of our formulas, we indicate how to derive the approximate functional equation for $\zeta^2(s)$ [3]. For simplicity we assume $p = q = 1$. Let $s = \sigma + it$, $\sigma \ge 0$, $t \ge 2$. Obviously, the second integral is sufficiently small, namely $\ll e^{-\frac{\pi t}{4}}$. Hence the main contribution comes from the first one. After a suitable modification of the path of integration, we arrive at

$$T(s) = \sum_{n \le t/2\pi} d(n)n^{-s} + \frac{\pi}{2i}\int_{z_0}^{z_1} \mathcal{G}^{(1)}(1,1,z)z^{1-s}\mathrm{d}z + O(e^{-ct}), \tag{3.5}$$

where $c > 0$ is a certain constant, and $z_{0,1} = \frac{t}{2\pi}(1 \mp \frac{1}{2}e^{\frac{\pi i}{4}})$. We modify the path so as to pass through the point $z = N + \frac{1}{2}$, where $N = [\frac{t}{2\pi}]$. Inserting the explicit formula (2.9) for $\mathcal{G}^{(1)}(1,1,z)$, and integrating term by term shows that the integral is $\ll t^{\sigma-\frac{1}{2}}\log t$. Hence

$$T(s) = \sum_{n \le t/2\pi} d(n)n^{-s} + O(t^{\sigma-\frac{1}{2}}\log t).$$

From Theorem 2 we finally get

$$\zeta^2(s) = \sum_{n \le t/2\pi} d(n)n^{-s} + \pi^{2s-1}X(s)\sum_{n \le t/2\pi} d(n)n^{s-1} + O(t^{\sigma-\frac{1}{2}}\log t),$$

which is the desired result. Choosing other values for p and q we obtain similarly an unsymmetric form of the approximate functional equation, where the ranges of summation are unequal (compare [6, III]). To derive a full asymptotic expansion of $T(s)$ (see [6, 7]), a detailed investigation of the integral in (3.5) is required, which is, however, the most difficult task. We shall return to this subject at another occasion.

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