A PARABOLIC CYLINDER FUNCTION
IN THE RIEMANN-SIEGEL INTEGRAL FORMULA

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Abstract. We show that the two integrals in the Riemann-Siegel integral formula can be transformed into integral representations that contain the parabolic cylinder function $U(a, z)$ as kernel function.

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1. INTRODUCTION

The Riemann-Siegel integral formula, first published by C. L. Siegel in 1932 (see [8, 9]), is the symmetric integral representation

$$\pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \zeta(s) = \mathcal{F}(s) + \mathcal{F}(1-s)$$

of Riemann’s zeta function where $s \in \mathbb{C}$ and

$$\mathcal{F}(s) := \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \int_{0}^{1} \frac{e^{i\pi u^2/2} e^{-s u}}{e^{i\pi u} - e^{-i\pi u}} \, du.$$ 

We will show that the function $\mathcal{F}(s)$ can be written in the form

$$\mathcal{F}(s) = 2^{s/2} \Gamma\left(\frac{s}{2}\right) e^{-i\pi(1-s)/4} \int_{-\frac{1}{\sqrt{2}}}^{\frac{1}{\sqrt{2}}} \frac{e^{-i\pi u^2/2 + i\pi u}}{2i \cos \pi u} U\left(s - 1/2, \sqrt{2\pi} e^{i\pi/4} u\right) \, du,$$

i.e., with an integral that contains the parabolic cylinder function $U(a, z)$ as kernel function.

In section 2 we present a real integral representation of $U(a, z)$ which is used in section 3. There we will see that the integral representation (1) is the consequence of the transformation of a special Mordell integral. The latter is proved in the appendix.

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We will use a notation of Siegel from [8, 9] here: Whenever there is an integration path with arrow, the path is a straight line of slope 1 or -1 from $\infty$ to $\infty$ in the direction of arrow crossing the real axis between the two points specified.

2. The Parabolic Cylinder Function

The parabolic cylinder function $U(a, z)$ can be defined by the contour integral

$$U(a, z) := \frac{\Gamma(1/2 - a)}{2\pi i} e^{-z^2/4} \int_C e^{-w^2/2 + zw} w^{a-1/2} dw \quad (a, z \in \mathbb{C}), \quad (2)$$

where the path $C$ comes from $\infty$ in the third quadrant parallel to the real axis, circles the origin once in the positive direction and returns to $\infty$ in the second quadrant parallel to the real axis again. $U(a, z)$ is an entire function of both variables and a solution of the differential equation $y'' - (z^2/4 + a) y = 0$. It satisfies a lot of recurrence relations such as

$$z U(a, z) - U(a - 1, z) + (a + 1/2) U(a + 1, z) = 0.$$  

We will show that the two integrals in the Riemann-Siegel integral formula (3) can be transformed into integrals that contain $U(a, z)$ as kernel function. For this we need

Theorem 2.1 (Real integral representation). If $a, z \in \mathbb{C}$ and $\Re(a) > -1/2$, we have

$$U(a, z) = e^{-z^2/4} \frac{\Gamma(1/2 - a)}{\Gamma(1/2 + a)} \int_0^\infty e^{-w^2/2 - zw} w^{a-1/2} dw.$$  

Proof. Let $\Re(a) > -1/2$ in (2). Then we can put the integration path on the real axis and through the origin giving

$$\int_C e^{-w^2/2 + zw} w^{a-1/2} dw = \int_{-\infty}^0 e^{-w^2/2 + zw + (a-1/2)[\log(-w) - i\pi]} dw + \int_{0}^\infty e^{-w^2/2 + zw + (a-1/2)[\log(-w) + i\pi]} dw$$

$$= [e^{-i\pi(a-1/2)} - e^{i\pi(a-1/2)}] \int_0^\infty e^{-w^2/2 - zw} w^{a-1/2} dw$$

$$= 2i \sin \pi \left(\frac{1}{2} - a\right) \int_0^\infty e^{-w^2/2 - zw} w^{a-1/2} dw.$$  

Therefore, the theorem follows from (2) by using the reflection formula of the gamma function.  

(1) See [1, 19.5.1].
(2) See [1, 19.6.4].
(3) To this formula see [4, 5, ch. 7], [8, 9] or [6, ch. 4, 4.1.1].
3. Transformation of the Riemann-Siegel Integral Formula

Setting \( \tau = 1 \) and \( x = z + 1/2 \) in the transformation formula of the Mordell integral (8), we obtain

\[
\int_{0}^{1} e^{i\pi u^2 + 2\pi i z u} du = \int_{0}^{1} e^{-i\pi u^2 + i\pi u} e^{-2\pi i u} e^{-i\pi z^2 + 2\pi i (u-1/2) z} du.
\]

We multiply this equation by \( z^{s-1} \) with \( s \) real > 1 and integrate over \( z \) along the bisecting line of the second quadrant. This yields for the left side of (3)

\[
e^{\frac{3\pi i}{4}} \int_{0}^{\infty} \int_{0}^{1} e^{-i\pi u^2 + i\pi u} e^{-2\pi i u} e^{-i\pi z^2 + 2\pi i (u-1/2) z} z^{s-1} du \cdot dz
\]

and for its right side

\[
e^{\frac{3\pi i}{4}} \int_{0}^{1} e^{-i\pi u^2 + i\pi u} e^{-2\pi i u} e^{-i\pi z^2 + 2\pi i (u-1/2) z} z^{s-1} du \int_{0}^{\infty} z^{s-1} dz
\]

\[
= (2\pi)^{-s/2} \Gamma(s) e^{3\pi s/4 + i\pi/8} \int_{0}^{\infty} e^{-i\pi u^2/2 + i\pi u/2} e^{-2\pi i u} U\left(s - 1/2, \sqrt{2\pi} e^{i\pi/4} (u - 1/2)\right) du,
\]

where we have used the formula

\[
e^{\frac{3\pi i}{4}} \int_{0}^{\infty} e^{-i\pi z^2 + 2\pi i (u-1/2) z} z^{s-1} dz
\]

\[
= (2\pi)^{-s/2} \Gamma(s) e^{3\pi s/4 + i\pi(u-1/2)^2/2} U\left(s - 1/2, \sqrt{2\pi} e^{i\pi/4} (u - 1/2)\right),
\]

which follows from theorem 2.1 if we substitute there \( w e^{3\pi i/4/\sqrt{2\pi}} \) for \( z \) in the integral. With these transformations from (3)

\[
\int_{0}^{1} e^{i\pi u^2} u^{s-1} du = \int_{0}^{1} e^{-i\pi u^2} u^{s-1} du
\]

\[
= (2\pi)^{s/2} e^{i\pi s/4 + i\pi/8} \int_{0}^{\infty} e^{-i\pi u^2/2 + i\pi u/2} e^{-2\pi i u} U\left(s - 1/2, \sqrt{2\pi} e^{i\pi/4} (u - 1/2)\right) du
\]

(4) The resulting double integrals converge absolutely so that the integration order can be interchanged. See also theorem [6, 4.1.6].
follows. Finally, if we substitute \( u + 1/2 \) for \( u \) in the last integral, we have

\[
\int_{0 \searrow 1} e^{i\pi u^2 u^{-s}} \frac{u^{-s}}{e^{i\pi u} - e^{-i\pi u}} \, du
\]

\[
= (2\pi)^{s/2} e^{i\pi (s+1)/4} \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{\frac{-i\pi u^2/2 + i\pi u}{2i \cos \pi u}} U\left(s - 1/2, \sqrt{2\pi} e^{i\pi/4} u\right) \, du
\]

and so

\[
\mathcal{F}(s) := \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \int_{0 \searrow 1} e^{i\pi u^2 u^{-s}} \frac{u^{-s}}{e^{i\pi u} - e^{-i\pi u}} \, du
\]

\[
= 2^{s/2} \Gamma\left(\frac{s}{2}\right) e^{-i\pi(1-s)/4} \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{\frac{-i\pi u^2/2 + i\pi u}{2i \cos \pi u}} U\left(s - 1/2, \sqrt{2\pi} e^{i\pi/4} u\right) \, du
\]

as well as

\[
\mathcal{F}(1-s) = \pi^{-(1-s)/2} \Gamma\left(\frac{1-s}{2}\right) \int_{0 \searrow 1} e^{i\pi u^2 u^{s-1}} \, du
\]

\[
= 2^{(1-s)/2} \Gamma\left(\frac{1-s}{2}\right) e^{i\pi s/4} \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{\frac{i\pi u^2/2 - i\pi u}{2i \cos \pi u}} U\left(1/2 - s, \sqrt{2\pi} e^{-i\pi/4} u\right) \, du,
\]

now valid for all \( s \) by analytic continuation. So the Riemann-Siegel integral formula

\[
\pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \zeta(s) = \mathcal{F}(s) + \mathcal{F}(1-s)
\]

yields an integral representation that contains the parabolic cylinder function \( U \) as integral kernel.

It should be noted that the cosine function on the right side of (4) is essential for the integral to converge in the second quadrant.

4. Appendix

We prove some theorems used above that are hard to find in the literature.

**Definition 4.1** (Mordell integral). For \( x, \tau \in \mathbb{C} \) and \( \Re(\tau) > 0 \) let

\[
\Phi(x, \tau) := \int_{0 \searrow 1} e^{i\pi x^2 + 2\pi i x u} \frac{e^{i\pi u^2} - 1}{e^{2\pi i u} - 1} \, du
\]

be a special Mordell integral\(^{(5)}\). The integration path is a straight line of slope 1 from the lower to the upper halfplane crossing the real axis between 0 and 1. \( \Phi(x, \tau) \) is an entire function of \( x \) because the integral converges regardless of the value of \( x \).

If \( \tau \) is a positive rational number, a representation of \( \Phi(x, \tau) \) using only exponential functions is given by

\(^{(5)}\) For definition and properties of Mordell integrals and their connection to theta functions see [7] and for some applications [6, ch. 4.1].
Theorem 4.1. Let \( m, n \) be natural numbers and \( \tau = m/n \). Then

\[
\Phi\left( x, m/n \right) = \sum_{k=1}^{n} e^{i\pi m/n k^2 + 2k\pi i/m} - \sqrt{m/n} e^{i\pi\left(1/4 - n/m x^2\right)} \sum_{k=1}^{m} e^{-i\pi n k^2 + 2k\pi i n x/m} e^{i\pi n(2x+m) - 1}. \tag{6}
\]

For a proof of this fundamental theorem see [2, ch. V] or [3, p. 35 ff.].

Theorem 4.2 (Functional equation of the Mordell integral). Let \( x, \tau \in \mathbb{C} \) and \( \Re(\tau) > 0 \). Then the functional equation

\[
\Phi(x, \tau) = -e^{i\pi\left(1/4 - x^2/\tau\right)} \sqrt{\tau} \Phi\left(-x/\tau, 1/\tau \right) \tag{7}
\]

and the integral transformation formula

\[
\int_{0 < u < 1} e^{i\pi u^2 + 2\pi i x u} e^{2\pi i u - 1} du = e^{i\pi\left(1/4 - x^2/\tau\right)} \int_{0 < u < 1} e^{-i\pi u^2/\tau + 2\pi i x u/\tau} e^{-2\pi i u - 1} du \tag{8}
\]

are valid.

Proof. We exchange \( n \) and \( m \) in (6). Then we replace \( x \) by \(-n\bar{x}/m\) and obtain

\[
\Phi\left(-n\bar{x}/m, m/n \right) = \sum_{k=1}^{m} e^{i\pi m/n k^2 - 2k\pi i/m} - \sqrt{m/n} e^{i\pi\left(1/4 - n/m x^2\right)} \sum_{k=1}^{n} e^{-i\pi n k^2 - 2k\pi i\bar{x}} e^{i\pi m(-2n\bar{x}/m + n) - 1}.
\]

Transition to the complex conjugated value yields

\[
\Phi\left(-n\bar{x}/m, m/n \right) = \sum_{k=1}^{m} e^{-i\pi n k^2 + 2k\pi i n x/m} - \sqrt{\tau} e^{-i\pi\left(1/4 - m/n x^2\right)} \sum_{k=1}^{n} e^{i\pi m k^2 + 2k\pi i x} e^{i\pi n(2x-m) - 1}.
\]

We multiply this equation by \(-\sqrt{m/n} e^{i\pi(1/4 - mx^2)/m}\) and regain the right side of (6) on the right side here since \( e^{i\pi n(2x-m)} = e^{i\pi n(2x+m)}\). Thus we have proved

\[
\Phi(x, \tau) = -e^{i\pi\left(1/4 - x^2/\tau\right)} \sqrt{\tau} \Phi\left(-\bar{x}/\tau, 1/\tau \right) \tag{9}
\]

if \( \tau = m/n \) is any positive rational number and \( x \in \mathbb{C} \). But since the rational numbers are dense in \( \mathbb{R} \), this equation must hold for all positive real numbers. Unfortunately, we cannot generalise this result to complex \( \tau \) directly because the complex conjugation is not a holomorphic operation. We use another way and replace \( \tau \) by \( 1/\tau \) and \( x \) by \(-\bar{x}/\tau\) in definition (5) giving

\[
\Phi\left(-\bar{x}/\tau, 1/\tau \right) = \int_{0 < u < 1} e^{i\pi u^2/\tau - 2\pi i u x/\tau} e^{2\pi i u - 1} du
\]

(6) Since \( \Phi(x, \tau) \) is an entire function of \( x \), every zero of the denominator must be also a zero of the numerator. From that we obtain interesting relations between exponential sums and an elegant proof of the quadratic reciprocity law (see [2, ch. V] or [3, p. 35 ff.]).
and therefore,

\[
\Phi\left(-\frac{x}{\tau}, \frac{1}{\tau}\right) = -\int_{0}^{\infty} \frac{e^{-i\pi u^2/\tau + 2\pi i xu/\tau}}{e^{-2\pi i u} - 1} \, du.
\]

We put this in (9) and under use of (5) we obtain the integral transformation formula (8) valid for positive real \(\tau\) and \(x \in \mathbb{C}\). Obviously, both sides of (8) are analytic functions of \(\tau\) if \(\Re(\tau) > 0\). So this equation holds for these \(\tau\) by analytic continuation as required. Finally, the functional equation (7) follows from (8) in combination with (5) because of

\[
\int_{0}^{\infty} \frac{e^{-i\pi u^2/\tau + 2\pi i xu/\tau}}{e^{-2\pi i u} - 1} \, du = \int_{0}^{\infty} \frac{e^{i\pi u^2/\tau - 2\pi i xu/\tau}}{e^{2\pi i u} - 1} \, du = -\Phi\left(-\frac{x}{\tau}, \frac{1}{\tau}\right).
\]

\(\square\)

Remark 1. The functional equation (7) differs only marginally from that of the Jacobian theta function \(\sum_{n=\pm \infty} e^{i\pi \tau n^2 + 2\pi i nx}(\Im(\tau) > 0)\). Indeed, Mordell has proved the strong connection between an integral like (5) and the theta functions in [7].

Remark 2. The integral transformation (8) can be used in the case of small \(|\tau|\) to convert a slowly convergent integral into a rapidly convergent one.

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