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AN ASYMPTOTIC EXPANSION FOR THE GENERALISED QUADRATIC GAUSS SUM REVISITED

R. B. PARIS

Abstract. An asymptotic expansion for the generalised quadratic Gauss sum

$$S_N(x,\theta)=\sum_{j=1}^{N}\exp(\pi ixj^2+2\pi ij\theta),$$

where x, θ are real and N is a positive integer, is obtained as $x\to 0$ and $N\to\infty$ such that Nx is finite. The form of this expansion holds for all values of $Nx+\theta$ and, in particular, in the neighbourhood of integer values of $Nx+\theta$. A simple bound for the remainder in the expansion is derived. Numerical results are presented to demonstrate the accuracy of the expansion and the sharpness of the bound.

1. Introduction

We consider the asymptotic expansion of the generalised quadratic Gauss sum

$$S_N(x,\theta)=\sum_{j=1}^{N}f(j),\quad f(t):=\exp(\pi ixt^2+2\pi i\theta t),\quad 0<x<1,\ -\tfrac{1}{2}\leqslant\theta\leqslant\tfrac{1}{2},\quad (1.1)$$

where N is a positive integer, as $x\to 0$ and $N\to\infty$, such that the quantity Nx is finite. Applications of the above exponential sum arise in various number-theoretic contexts and in the study of disorder in dynamical systems.

The sum $S_N(x,\theta)$ has a long history that goes back to Gauss, who evaluated the sum corresponding to $x=2/N$ when $\theta=0$. The results of Gauss were generalised for rational $x=M/N$, where M and N are relatively prime, into the well-known Cauchy-Kronecker formula [1]

$$S_N(x,0)=\frac{e^{\pi i/4}}{\sqrt{x}}S_M\left(-\frac{1}{x},0\right)\qquad (x=M/N,\ MN\text{ even}).$$

When its terms are regarded as unit vectors in the complex plane, the patterns produced by the partial sums of (1.1) for fixed x as $N\to\infty$ often result in a superposition of spirals (or "curlicues") that can be highly intricate; see [2, 3, 4, 9]. The scalings of this hierarchy of spirals are found to depend delicately on the arithmetic nature of x [3]. When $x=p/q$, where p and q are relatively prime, and $\theta=0$ the trace is relatively simple: when pq is even the spiral pattern is regular and 'diffuses' in the complex

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plane away from the origin in blocks, whereas when pq is odd the pattern is periodic and repeats itself indefinitely as $N \to \infty$. When x is irrational a more complicated pattern emerges that seems to exhibit a random-walk behaviour; see [3, 12].

Estimates for the growth of $S_N(x,\theta)$ when N is large and x is fixed in the range $0 < x < 1$ are obtained by employing a renormalisation process based on the approximate functional relation [7]

$$S_N(x,\theta) = \frac{e^{-\pi i\theta^2/x+\pi i/4}}{\sqrt{x}} S_{\lfloor Nx \rfloor}\left(-\frac{1}{x}, \frac{\theta}{x}\right) + O\left(\frac{1+|\theta|}{\sqrt{x}}\right). \tag{1.2}$$

This transformation shows that the sum $S_N(x,\theta)$ over N terms can be approximated by a similar sum taken over $\lfloor Nx \rfloor$ terms with the variable x replaced by $-1/x$ and θ by θ/x. Repeated application of (1.2), making use of the simple symmetry properties satisfied by (1.1) to maintain x in the interval $0 < x < 1$ at each stage, enables the representation of $S_N(x,\theta)$ in terms of a steadily decreasing number of terms. In this way it was shown in [7] that $S_N(x,\theta) = o(N)$ for any irrational x, with more precise order estimates depending on the detailed arithmetic structure of x.

The problem that concerns us here is the asymptotic estimation of $S_N(x,\theta)$ for $x \to 0$ when $N \to \infty$ such that Nx is finite. An early paper dealing with estimates for $S_N(x,\theta)$ when $0 < x < 1$ is that of Fiedler *et al.* [6], and more recently that in [8, §2.2], but their error terms are too large for our purposes when $x \to 0$. Following on from the gross estimates in [9], the leading terms in the expansion in the case $\theta = 0$ were obtained in [13] when $Nx < 1$. An expansion for $S_N(x,0)$ valid as $x \to 0$ and finite Nx was obtained in [3] and [5, Theorem 4], although the remainder term was left as an order estimate.

In this paper, we revisit the expansion of $S_N(x,\theta)$ as $x \to 0$ and $N \to \infty$ such that $Nx = O(1)$ obtained in [12]. The sum $S_N(x,\theta)$ is expressed exactly as a series of complementary error functions with argument proportional to $x^{-1/2}$, so that in the small-x limit we may employ the well-known asymptotics of the complementary error function in the form [11, §7.12(i)]

$$e^{z^2}\operatorname{erfc}(z) = \frac{1}{\sqrt{\pi}} \sum_{r=0}^{n-1} (-)^r \frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})} z^{-2r-1} + \hat{T}_n(z) \qquad (|z| \to \infty), \tag{1.3}$$

where

$$|\hat{T}_n(z)| \leqslant \frac{\Gamma(n+\frac{1}{2})}{\pi} |z|^{-2n-1} \qquad (|\arg z| \leqslant \tfrac{1}{4}\pi) \tag{1.4}$$

and n is a positive integer; see also [10, p. 111]. In [12], the coefficients in the resulting expansion were expressed in terms of even-order derivatives of $\cot \pi\xi$, where $\xi = Nx + \theta$, which presented a complication when ξ passes through integer values. In addition, the remainder in the expansion was not expressed as a convenient bound. Here we remedy these deficiencies and give the expansion in a form with coefficients that do not present any difficulty in computation in the neighbourhood of integer values of ξ.

In order to make the paper reasonably self-contained, we repeat in Section 2 the derivation of the representation of $S_N(x,\theta)$ in terms of complementary error functions given in [12]. In Section 3, we establish the central result of the paper in the following theorem.

THEOREM 1. *Let $S_N(x,\theta)$ be the sum defined in (1.1), where $0<x<1$, $-\frac{1}{2}\leqslant\theta\leqslant\frac{1}{2}$ and N is a positive integer. Further, let $\xi := Nx+\theta$, $M=[\xi]$ be the nearest integer part of ξ and $\varepsilon := \xi - M$, where $-\frac{1}{2}<\varepsilon\leqslant\frac{1}{2}$. Then, as $x\to 0$ and $N\to\infty$, such that Nx is finite, we have the expansion valid for $M\geqslant 0$ and $n\geqslant 1$*

$$S_N(x,\theta)-\frac{e^{-\pi i\theta^2/x+\pi i/4}}{\sqrt{x}}S_M\left(-\frac{1}{x},\frac{\theta}{x}\right)-\frac{1}{2}(f(N)-1)$$
$$-\frac{e^{\pi i/4}}{2\sqrt{x}}\{E(\theta)-f(N)E(\varepsilon)\}=\frac{1}{2\pi i}\sum_{r=0}^{n-1}\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}\left(\frac{x}{\pi i}\right)^r C_r+R_n, \tag{1.5}$$

where $E(t):=e^{-\pi it^2/x}\,\mathrm{erfc}\,(e^{\pi i/4}t\sqrt{\pi/x})$. The coefficients C_r are given by

$$C_r=f(N)\Delta_r^-(\varepsilon)-\Delta_r^-(\theta)\qquad(r\geqslant 0) \tag{1.6}$$

and the remainder R_n satisfies the bound

$$|R_n|\leqslant\frac{(\frac{1}{2})_n}{2\pi}\left(\frac{x}{\pi}\right)^n(\Delta_n^+(\varepsilon)+\Delta_n^+(\theta))\qquad(n\geqslant 1), \tag{1.7}$$

where the quantities $\Delta_r^\pm(\lambda)$ are defined in (3.1) and (3.2).

In Section 4, we present numerical results to demonstrate the accuracy of the above expansion and also the sharpness of the bound on the remainder term R_n.

2. A representation for $S_N(x,\theta)$

Let $\xi := Nx+\theta$, $M=[\xi]$, $\varepsilon=\xi-[\xi]$, where $[\xi]$ denotes the *nearest* integer part of ξ and $-\frac{1}{2}<\varepsilon\leqslant\frac{1}{2}$. Define also the function

$$E(t):=e^{-\pi it^2/x}\,\mathrm{erfc}\,(\omega t\sqrt{\pi/x}),\qquad \omega=e^{-\pi i/4},$$
$$E(0)=1,\qquad E(-t)=2e^{-\pi it^2/x}-E(t), \tag{2.1}$$

where erfc is the complementary error function. The reflection formula follows from the well-known result $\mathrm{erfc}\,(z)=2-\mathrm{erfc}\,(-z)$. From (1.3), we have the expansion for $x^{-1/2}t\to+\infty$

$$E(t)=\frac{1}{\sqrt{\pi}}\sum_{r=0}^{n-1}(-)^r\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}\left(\frac{ix}{\pi t^2}\right)^{r+\frac{1}{2}}+T_n(t)\qquad(n=1,2,\ldots), \tag{2.2}$$

where from (1.4)

$$|T_n(t)| \leqslant \frac{\Gamma(n+\frac{1}{2})}{\pi}\left(\frac{x}{\pi t^2}\right)^{n+\frac{1}{2}}. \tag{2.3}$$

An application of Cauchy's theorem shows that

$$\sum_{j=1}^{N-1} f(j) = \frac{1}{2i}\int_{\mathscr{C}} \cot(\pi t) f(t)\,dt,$$

where $f(t)$ is defined in (1.1) and $\mathscr{C}$ is a closed path encircling only the poles of the integrand at $t = 1, 2, \ldots, N-1$. We deform the path $\mathscr{C}$ into a parallelogram with two sides inclined at $\frac{1}{4}\pi$ to the real axis; see [12]. The vertices are situated at $\pm Pe^{\pi i/4}$, $N \pm Pe^{\pi i/4}$ $(P > 0)$ and there are semi-circular indentations of radius $\delta < 1$ around the points $t = 0$ and $t = N$. Then, denoting the upper and lower halves of the contour by $\mathscr{C}_1$ and $\mathscr{C}_2$ respectively, we find following the discussion given in [10, p. 290] that

$$\sum_{j=1}^{N-1} f(j) = \int_{\delta}^{N-\delta} f(t)\,dt + \int_{\mathscr{C}_1} \frac{f(t)}{1-e^{-2\pi i t}}dt + \int_{\mathscr{C}_2} \frac{f(t)}{e^{2\pi i t}-1}dt.$$

Now let $P \to \infty$, so that the contributions from the parts of $\mathscr{C}_1$ and $\mathscr{C}_2$ parallel to the real axis vanish on account of the exponential decay of the factor $\exp(\pi i x t^2)$, and let $\delta \to 0$. The integrals around the indentation linking $\delta e^{\pi i/4}$ with δ and δ with $-\delta e^{\pi i/4}$ then tend to $-\frac{1}{8}f(0)$ and $-\frac{3}{8}f(0)$, respectively; similarly for the indentation at $t = N$ the integrals contribute $\frac{1}{2}f(N)$. Thus we obtain

$$S_N(x,\theta) = \sum_{j=1}^{N} f(j) = \tfrac{1}{2}(f(N)-1) + J_N + e^{\pi i/4}(I_N - I_0), \tag{2.4}$$

where the integral

$$J_N := \int_0^N f(t)\,dt = \frac{e^{\pi i/4}}{2\sqrt{x}}\{E(\theta) - f(N)E(\xi)\} \tag{2.5}$$

and we have defined

$$I_j := \int_0^\infty \frac{F_j(\tau)}{e^{2\pi\omega\tau}-1}d\tau \qquad (j = 0, N)$$

with

$$F_j(\tau) := f(j - \tau e^{\pi i/4}) - f(j + \tau e^{\pi i/4}) = 2e^{-\pi x\tau^2} f(j)\sinh\{2\pi(jx+\theta)\omega\tau\}.$$

It now remains to evaluate the integrals I_0 and I_N. If we expand the factor $(e^{2\pi\omega\tau}-1)^{-1}$ as a finite geometric series together with a remainder we find, for positive integer K,

$$I_j = \sum_{k=1}^{K}\int_0^\infty e^{-2\pi k\omega\tau} F_j(\tau)\,d\tau + \int_0^\infty \frac{e^{-2\pi K\omega\tau} F_j(\tau)}{e^{2\pi\omega\tau}-1}d\tau. \tag{2.6}$$

The first term on the left-hand side of this expression becomes upon insertion of the definition of $F_j(\tau)$

$$2f(j)\sum_{k=1}^{K}\int_0^\infty e^{-\pi x\tau^2-2\pi k\omega\tau}\sinh\{2\pi(jx+\theta)\omega\tau\}\,d\tau$$

$$=\frac{f(j)}{2\sqrt{x}}\sum_{k=1}^{K}\{E(k-jx-\theta)-E(k+jx+\theta)\}. \quad (2.7)$$

The remainder term in (2.6) is given by

$$H_K:=\int_0^\infty \frac{e^{-2\pi K\omega\tau}F_j(\tau)}{e^{2\pi\omega\tau}-1}d\tau=f(j)\int_0^\infty e^{-\pi\tau(x\tau+\omega)}e^{-2\pi(K-jx-\theta)\omega\tau}G(\tau)\,d\tau,$$

where

$$G(\tau):=e^{-2\pi(jx+\theta)\omega\tau}\sinh\{2\pi(jx+\theta)\omega\tau\}/\sinh(\pi\omega\tau).$$

Now $G(0)=2(jx+\theta)$ and $G(\tau)\sim e^{-\pi\omega\tau}$ as $\tau\to+\infty$. It is also easy to see (we omit these details) that $|G(\tau)|\leqslant G(0)$ for $\tau\in[0,\infty)$. Then, provided $K>jx+\theta$ $(j=0,N)$ it follows that

$$|H_K|<\int_0^\infty e^{-2\pi(K-jx-\theta)\omega_r\tau}|G(\tau)|\,d\tau\leqslant\frac{2^{\frac{1}{2}}G(0)}{2\pi(K-jx-\theta)}$$

where $\omega_r=1/\sqrt{2}$, with the result that $H_K\to 0$ as $K\to\infty$. Therefore, from (2.7), we obtain

$$I_j=\frac{f(j)}{2\sqrt{x}}\sum_{k=1}^{\infty}\{E(k-jx-\theta)-E(k+jx+\theta)\}\qquad(j=0,N). \quad (2.8)$$

From (2.2) we see that the terms in (2.8) are $O(k^{-2})$ as $k\to\infty$.

Substitution of (2.8) with $j=0$ and $j=N$ into (2.4), together with (2.5), then yields the desired representation of $S_N(x,\theta)$ in terms of complementary error functions.

3. The expansion of $S_N(x,\theta)$ as $x\to 0$ with Nx finite

We define the quantities for $|\lambda|<1$

$$\Delta_r^+(\lambda):=\zeta(2r+1,1+\lambda)+\zeta(2r+1,1-\lambda)\quad(r\geqslant 1), \quad (3.1)$$

and

$$\Delta_r^-(\lambda):=\begin{cases}\pi\cot\pi\lambda-\lambda^{-1} & (r=0)\\ \zeta(2r+1,1+\lambda)-\zeta(2r+1,1-\lambda) & (r\geqslant 1),\end{cases} \quad (3.2)$$

where $\zeta(s,a)=\sum_{k=0}^\infty(k+a)^{-s}$ $(\Re(s)>1)$ is the Hurwitz zeta function. Note that $\Delta_r^-(0)=0$ for $r\geqslant 0$ and $\Delta_r^+(0)=2\zeta(2r+1)$, where $\zeta(s)$ is the Riemann zeta function.

When $j=0$, we have from (2.8)

$$I_0=\frac{1}{2\sqrt{x}}\sum_{k=1}^{\infty}\{E(k-\theta)-E(k+\theta)\}.$$

In the limit $x\to 0$, the arguments of the complementary error functions contained in $E(k\pm\theta)$ have large modulus for $k\geqslant 1$ and phase equal to $-\frac{1}{4}\pi$, since $-\frac{1}{2}\leqslant\theta\leqslant\frac{1}{2}$. Employing the expansion (2.2), we then obtain

$$I_0=-\frac{e^{\pi i/4}}{2\pi}\sum_{r=1}^{n-1}\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}\left(\frac{x}{\pi i}\right)^r c_r(\theta)+\mathscr{R}_n(\theta)\qquad(x\to 0),\tag{3.3}$$

where

$$\begin{aligned}c_r(\theta)=\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}(k+\theta)^{-2r-1}&=\sum_{k=0}^{\infty}(k+1+\theta)^{-2r-1}-\sum_{k=0}^{\infty}(k+1-\theta)^{-2r-1}\\&=\Delta_r^-(\theta).\end{aligned}\tag{3.4}$$

In the case $r=0$ the sums must be interpreted in the principal value sense $\lim_{s\to\infty}\sum_{k=-s}^{s}a_k$ to yield the evaluation $c_0(\theta)=\pi\cot\pi\theta-1/\theta$. The remainder term $\mathscr{R}_n(\theta)$ is given by

$$\mathscr{R}_n(\theta)=\frac{1}{2\sqrt{x}}\sum_{k=1}^{\infty}\{T_n(k-\theta)-T_n(k+\theta)\}$$

and, from (2.3), therefore satisfies the bound

$$|\mathscr{R}_n(\theta)|\leqslant\frac{(\frac{1}{2})_n}{2\pi}\left(\frac{x}{\pi}\right)^n\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}|k+\theta|^{-2n-1}=\frac{(\frac{1}{2})_n}{2\pi}\left(\frac{x}{\pi}\right)^n\Delta_n^+(\theta),\tag{3.5}$$

where $(a)_r=\Gamma(a+r)/\Gamma(a)$ is the Pochhammer symbol.

Proceeding in a similar manner when $j=N$, we have

$$\begin{aligned}I_N&=\frac{f(N)}{2\sqrt{x}}\sum_{k=1}^{\infty}\{E(k-\xi)-E(k+\xi)\}\\&=\frac{f(N)}{2\sqrt{x}}\left\{\sum_{k=1}^{M}\{2e^{-\pi i(k-\xi)^2/x}-E(\xi-k)\}+\sum_{k=M+1}^{\infty}E(k-\xi)-\sum_{k=1}^{\infty}E(k+\xi)\right\}.\end{aligned}$$

Here we have made use of the reflection formula in (2.1) to separate off the error functions in $E(k-\xi)$ corresponding to $k\leqslant M$ (when $M\geqslant 1$). Upon noting that

$$f(N)e^{-\pi i(k-\xi)^2/x}=e^{-\pi i\theta^2/x}e^{-\pi ik^2/x+2\pi ki\theta/x},$$

we obtain when $M\geqslant 1$

$$I_N=\frac{e^{-\pi i\theta^2/x}}{\sqrt{x}}S_M\left(-\frac{1}{x},\frac{\theta}{x}\right)-\frac{f(N)}{2\sqrt{x}}\left\{\sum_{k=1}^{\infty}E(k+\xi)+\sum_{k=1}^{M}E(\xi-k)-\sum_{k=M+1}^{\infty}E(k-\xi)\right\}.\tag{3.6}$$

If we now extract from the second sum in curly braces in (3.6) the error function $E(\xi-k)$ corresponding to $k=M$ (that is, $E(\varepsilon)$) and use the evaluation of the integral J_N in (2.5), we can write

$$e^{\pi i/4}I_N+J_N=\frac{e^{-\pi i\theta^2/x+\pi i/4}}{\sqrt{x}}S_M\left(-\frac{1}{x},\frac{\theta}{x}\right)+\frac{e^{\pi i/4}}{2\sqrt{x}}\{E(\theta)-f(N)E(\varepsilon)\}$$
$$-\frac{e^{\pi i/4}f(N)}{2\sqrt{x}}\left\{\sum_{k=0}^{\infty}E(k+\xi)+\sum_{k=1}^{M-1}E(\xi-k)-\sum_{k=M+1}^{\infty}E(k-\xi)\right\},\quad(3.7)$$

where the term involving $f(N)E(\xi)$ from J_N has been absorbed into the first sum in curly braces.

Then in a similar manner to the determination of the expansion of I_0 in (3.3) we find

$$\frac{1}{2\sqrt{x}}\left\{\sum_{k=0}^{\infty}E(k+\xi)+\sum_{k=1}^{M-1}E(\xi-k)-\sum_{k=M+1}^{\infty}E(k-\xi)\right\}$$
$$=\frac{e^{\pi i/4}}{2\pi}\sum_{r=0}^{n-1}\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}\left(\frac{x}{\pi i}\right)^r c_r(\varepsilon)+\mathscr{R}_n(\varepsilon),\quad(3.8)$$

where, recalling that $\xi=M+\varepsilon$, $M=[\xi]$,

$$c_r(\varepsilon)=\sum_{\substack{k=-\infty\\k\neq -M}}^{\infty}(k+\xi)^{-2r-1}=\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}(k+\varepsilon)^{-2r-1}=\Delta_r^-(\varepsilon)\quad(3.9)$$

and the remainder $\mathscr{R}_n(\varepsilon)$ satisfies the bound

$$|\mathscr{R}_n(\varepsilon)|\leqslant\frac{(\frac{1}{2})_n}{2\pi}\left(\frac{x}{\pi}\right)^n\sum_{\substack{k=-\infty\\k\neq -M}}^{\infty}|k+\xi|^{-2n-1}=\frac{(\frac{1}{2})_n}{2\pi}\left(\frac{x}{\pi}\right)^n\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}|k+\varepsilon|^{-2n-1}$$
$$=\frac{(\frac{1}{2})_n}{2\pi}\left(\frac{x}{\pi}\right)^n\Delta_n^+(\varepsilon).\quad(3.10)$$

Combination of (3.7) and (3.8) then yields the expansion when $M\geqslant 1$

$$e^{\pi i/4}I_N+J_N=\frac{e^{-\pi i\theta^2/x+\pi i/4}}{\sqrt{x}}S_M\left(-\frac{1}{x},\frac{\theta}{x}\right)+\frac{e^{\pi i/4}}{2\sqrt{x}}\{E(\theta)-f(N)E(\varepsilon)\}$$
$$+\frac{1}{2\pi i}\sum_{r=0}^{n-1}\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}\left(\frac{x}{\pi i}\right)^r c_r(\varepsilon)+\mathscr{R}_n(\varepsilon).\quad(3.11)$$

In the case $M=0$ (when $\xi=\varepsilon$), the sum $S_M\equiv 0$ and from (3.6) we have

$$e^{\pi i/4}I_N+J_N=\frac{e^{\pi i/4}}{2\sqrt{x}}\{E(\theta)-f(N)E(\varepsilon)\}-\frac{e^{\pi i/4}f(N)}{2\sqrt{x}}\left\{\sum_{k=1}^{\infty}E(k+\varepsilon)-\sum_{k=1}^{\infty}E(k-\varepsilon)\right\}.$$

It is easily seen that we obtain the same expansion as (3.11).

The form of the coefficients in (3.4) and (3.9) with $r \geqslant 1$ presents no difficulty in computation in the neighbourhood of integer values of ξ where $\varepsilon \simeq 0$, in contrast to those given in [12] which involved even derivatives of $\cot \pi\xi$. Although the coefficients $c_0(\varepsilon)$ and $c_0(\theta)$ have a removable singularity at $\varepsilon = 0$ and $\theta = 0$ their computation is straightforward.

If we now define the coefficients C_r and the remainder R_n by

$$C_r := f(N)c_r(\varepsilon) - c_r(\theta), \qquad R_n := e^{\pi i/4}\{f(N)\mathscr{R}_n(\varepsilon) - \mathscr{R}_n(\theta)\},$$

then we see that

$$C_r = f(N)\Delta_r^-(\varepsilon) - \Delta_r^-(\theta) \quad (r \geqslant 0) \tag{3.12}$$

and

$$|R_n| \leqslant |\mathscr{R}_n(\varepsilon)| + |\mathscr{R}_n(\theta)| \leqslant \frac{(\frac{1}{2})_n}{2\pi}\left(\frac{x}{\pi}\right)^n \{\Delta_n^+(\varepsilon) + \Delta_n^+(\theta)\} \quad (n \geqslant 1). \tag{3.13}$$

Combination of (2.4), (3.3) and (3.11), together with the above definitions of C_r and the bound on R_n, then gives the expansion of $S_N(x,\theta)$ stated in Theorem 1. We remark that the terms $E(\theta)$ and $E(\varepsilon)$ have been left unexpanded as $x \to 0$ in (3.11) and in Theorem 1, since for small values of θ and $\varepsilon = o(x^{1/2})$ these quantities can no longer be approximated by (2.2).

4. Numerical results and discussion

In order to demonstrate the accuracy of the expansion in Theorem 1, we define the quantity $\mathscr{S}$ by

$$\mathscr{S} := S_N(x,\theta) - \frac{e^{-\pi i\theta^2/x + \pi i/4}}{\sqrt{x}} S_M\left(-\frac{1}{x}, \frac{\theta}{x}\right) - \frac{1}{2}(f(N)-1) - \frac{e^{\pi i/4}}{2\sqrt{x}}\{E(\theta) - f(N)E(\varepsilon)\}. \tag{4.1}$$

Then from Theorem 1 we have the expansion as $x \to 0$ and $N \to \infty$ such that Nx is finite

$$\mathscr{S} = \frac{1}{2\pi i}\sum_{r=0}^{n-1} \frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}\left(\frac{x}{\pi i}\right)^r C_r + R_n, \tag{4.2}$$

where the coefficients C_r are defined in (1.6) and the remainder R_n satisfies the bound in (1.7). We remark that the bound in (1.7) is explicitly independent of N. In Table 1, we show the absolute value of the error in the computation of $\mathscr{S}$ using the expansion (4.2) truncated after n terms for two different sets of values of x, θ, summation index N and different levels n. The exact value of $S_N(x,\theta)$ was obtained by high-precision summation of (1.1). In Table 2, we compare the absolute values of the remainder R_n calculated from (4.2) and its bound to illustrate the sharpness of (1.7).

In the case of the classical quadratic Gauss sum ($\theta = 0$), we have $\xi = Nx = M + \varepsilon$ with $-\frac{1}{2} < \varepsilon \leqslant \frac{1}{2}$ (when $M \geqslant 1$). From (1.5) as $x \to 0$, $N \to \infty$ such that Nx is finite,

Table 1: *Values of the absolute error in the computation of $\mathscr{S}$ by (4.2) for different truncation index n.*

n	$x=1/(250\sqrt{\pi})$ $N=7300,\ \theta=-0.125$ $\xi \doteq 16.349$	$x=1/(250\sqrt{\pi})$ $N=7430,\ \theta=0.25$ $\xi \doteq 17.018$	$x=1/(250\sqrt{3})$ $N=6000,\ \theta=0$ $\xi \doteq 6.928$
1	2.216×10^{-4}	1.198×10^{-4}	1.386×10^{-5}
2	5.642×10^{-7}	2.527×10^{-7}	1.221×10^{-8}
3	2.346×10^{-9}	8.332×10^{-10}	1.590×10^{-11}
4	1.369×10^{-11}	3.752×10^{-12}	2.708×10^{-14}
6	9.569×10^{-16}	1.509×10^{-16}	1.420×10^{-19}
8	1.334×10^{-19}	1.194×10^{-20}	1.360×10^{-24}
10	3.096×10^{-23}	1.568×10^{-24}	2.082×10^{-29}

Table 2: *The absolute values of R_n and the bound in (1.7) for different truncation index n.*

n	$x=1/(250\sqrt{\pi}),\ \theta=-0.125$ $N=7300,\ \xi \doteq 16.349$		$x=1/(250\sqrt{\pi}),\ \theta=0.25$ $N=7430,\ \xi \doteq 17.018$	
	$\lvert R_n\rvert$	Bound	$\lvert R_n\rvert$	Bound
1	2.216×10^{-4}	4.062×10^{-4}	1.200×10^{-4}	3.272×10^{-4}
2	5.642×10^{-7}	7.077×10^{-7}	2.527×10^{-7}	4.137×10^{-7}
4	1.369×10^{-11}	1.435×10^{-11}	3.752×10^{-12}	4.309×10^{-12}
6	9.569×10^{-16}	9.691×10^{-16}	1.509×10^{-16}	1.570×10^{-16}
8	1.334×10^{-19}	1.339×10^{-19}	1.194×10^{-20}	1.208×10^{-20}
10	3.096×10^{-23}	3.100×10^{-23}	1.568×10^{-24}	1.574×10^{-24}

we obtain the expansion

$$S_N(x,0)=\frac{e^{\pi i/4}}{\sqrt{x}}S_M\left(-\frac{1}{x},0\right)+\frac{1}{2}(f(N)-1)+\frac{e^{\pi i/4}}{2\sqrt{x}}\{1-f(N)E(\varepsilon)\}$$
$$+\frac{f(N)}{2\pi i}\sum_{r=0}^{n-1}\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}\left(\frac{x}{\pi i}\right)^r c_r(\varepsilon)+R_n', \tag{4.3}$$

where $f(N)=\exp(\pi i x N^2)$. From (1.7) and the fact that $I_0\equiv 0$ when $\theta=0$, we have

$$|R_n'|\leqslant\frac{(\frac{1}{2})_n}{2\pi}\left(\frac{x}{\pi}\right)^n\Delta_n^+(\varepsilon). \tag{4.4}$$

We emphasise that the expansion in (4.3) holds for all finite values of Nx; see Table 1. When $M=[\xi]=0$ and $0<\varepsilon\leqslant\frac{1}{2}$ — that is, when $Nx<\frac{1}{2}$ — the sum $S_M=$

0. If, in addition, $E(\varepsilon)$ in (4.3) is expanded by means of (2.2) then we obtain an expansion equivalent to that in [5, Theorem 4], albeit with a bound for the remainder rather than an order estimate and coefficients c_r expressed in a different form. However, the expansion of $E(\varepsilon)$ by (2.2) is only applicable when $\varepsilon \gg x^{1/2}$; that is, when $N \gg x^{-1/2}$.

Finally, we remark that since $C_r \sim (1-|\varepsilon|)^{-2r-1}$ for $r \gg 1$ (when ε is bounded away from zero), the optimal truncation index r_0 of the sum in (4.2) (corresponding to truncation at, or near, the term of least magnitude) is given by $r_0 \simeq \pi(1-|\varepsilon|)^2/x$. This shows that the values of the truncation index n in Table 1 are highly sub-optimal and also gives an indication of the enormous accuracy that could be obtained from the expansion (4.2).

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R. B. Paris
School of Engineering, Computing and Applied Mathematics
University of Abertay Dundee
Dundee DD1 1HG, UK