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An Asymptotic Expansion for the Generalised Quadratic Gauss Sum

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Abstract

An asymptotic expansion for the generalised quadratic Gauss sum $S_N(x,\theta)=\sum_{j=0}^N \exp(\pi ixj^2+2\pi ij\theta)$, where x, θ are real and N is a positive integer, is obtained as $x\to 0$ and $N\to\infty$ such that $Nx=O(1)$. A modified form of this expansion is given that holds in the neighbourhood of integer values of $Nx+\theta$. Numerical results are presented to demonstrate the accuracy of the expansions.

Keywords: Quadratic Gauss sum; Exponential sums; Asymptotics; Curlicues

1. Introduction

We consider the generalised quadratic Gauss sum

$$S_N(x,\theta)=\sum_{j=0}^{N}{}' \exp(\pi ixj^2+2\pi ij\theta), \tag{1.1}$$

where $0<x<1$, $-\frac{1}{2}\leq\theta\leq\frac{1}{2}$ and N is a positive integer. The prime on the sum indicates that the first and last terms are halved. Our interest in this paper is concerned with obtaining an asymptotic expansion for $S_N(x,\theta)$ as $x\to 0$ and $N\to\infty$, such that the quantity $Nx=O(1)$. Applications of the above exponential sum arise in various number-theoretic contexts and in the study of disorder in dynamical systems. Two physical applications when $\theta=0$ arising in quantum spin in an axially symmetric electric field and in Fresnel diffraction from large gratings are discussed in [2].

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 $x = p/q$, where p and q are relatively prime, into the elegant formula established by Genocchi and Schaar [12]

$$S_q(p/q, 0) = e^{\pi i/4}(q/p)^{\frac{1}{2}} S_p(-q/p, 0)$$

when pq is even. An investigation of Gauss sums $S_N(2/q, 0)$ with $N < \frac{1}{2}q$ was undertaken in [13], where best possible estimates for the maximum modulus were obtained. The geometric content of the sum $S_N(x, 0)$ was first highlighted in [5, 13] and subsequently explored in [2, 3]. The spiralling patterns produced by the partial sums of (1.1) (when its terms are regarded as unit vectors in the complex plane) for fixed x as $N \to \infty$ can result in an intricate pattern consisting of a superposition of spirals (or "curlicues"). The scalings of this hierarchy of spirals is found to depend delicately on the arithmetic nature of x [2, 3]. When $x = p/q$, where p and q are relatively prime, and $\theta = 0$ the trace of the partial sums of (1.1) is relatively simple. When pq is even the spiral pattern is regular and 'diffuses' in the complex plane away from the origin in blocks, while when pq is odd the pattern is periodic and repeats itself indefinitely as $N \to \infty$. Accordingly, $S_N(x, 0) = O(N)$ or $O(1)$ as $N \to \infty$ when pq is even or odd. When x is irrational a more complicated pattern emerges with the pattern exhibiting a seemingly random-walk behaviour; see Fig. 1.

Estimates for the growth of $S_N(x, \theta)$ when N is large and x is fixed in the range $0 < x < 1$ were considered in [8] using a renormalisation process (which is related to the Poisson summation formula). The fundamental tool in this analysis is the approximate functional relation [7, 8]

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

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 that $S_N(x, \theta) = o(N)$ for any irrational x, with more precise order estimates depending on the detailed arithmetic structure of x [8].

A different problem, which 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*

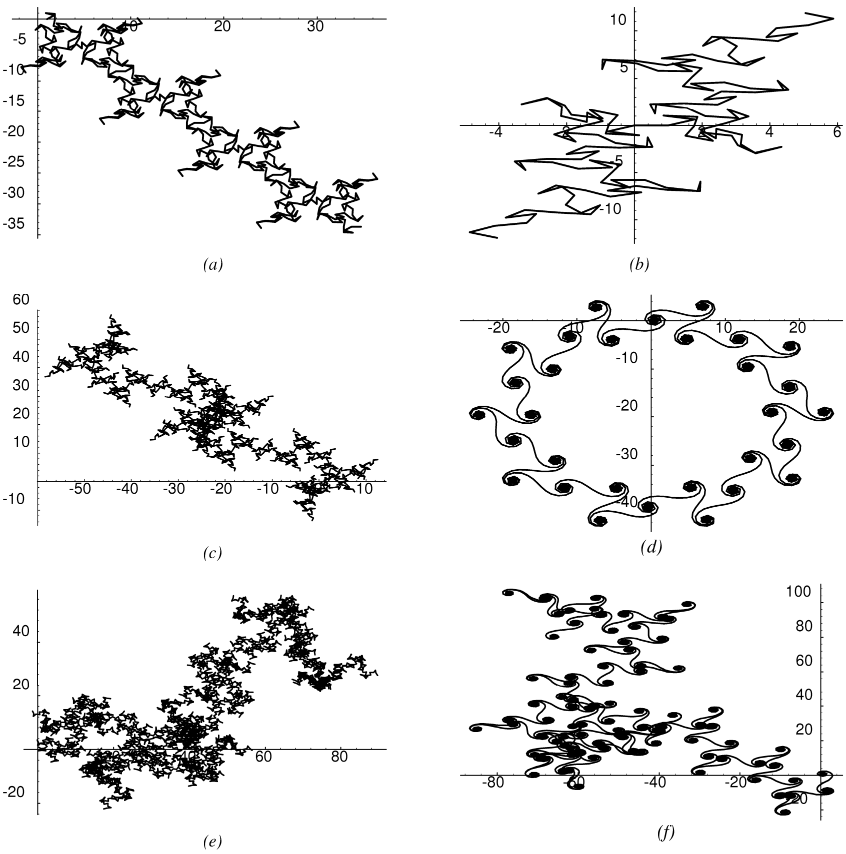

Figure 1: Traces of the partial sums of (1.1) in the complex plane when (a) $x = 31/142$, $\theta = 0$ (b) $x = 31/143$, $\theta = 0$ (c) $x = 707/1000$, $\theta = 0$ with $N \leq 2 \times 10^3$, (d) $x = 3/151$, $\theta = 0.4$, (e) $x = 5^{-1/2}$, $\theta = 0$ with $N \leq 5 \times 10^3$ and (f) $x = 1/(50\sqrt{\pi})$, $\theta = 0.2$ with $N \leq 8 \times 10^3$. The patterns in (a) and (c) diffuse away from the origin in periodic blocks of 142 and 10^3 terms, respectively; the figures show 4 such blocks in (a) and 2 blocks in (c). The pattern in (b) is periodic with period $2 \times 143 = 286$. In (e) and (f) the pattern exhibits a random-walk behaviour typical of irrational x.

al. [7], and more recently that in [10, §2.2], but their error terms are too large for our purposes when $x \to 0$. Following on from the gross estimates in [13], the leading terms in the expansion in the case $\theta = 0$ were obtained in [17] when $Nx < 1$. Asymptotic expansions of the higher-order Gauss sum $\sum_{j=0}^{N} \exp(\pi i x j^p)$ valid as $x \to 0$ in the principal spiral $pxN^{p-1}/2 < 1$ have been given in [6, 15]. In the special case $p = 2$, however, the expansions so obtained also only described the asymptotic structure of $S_N(x, 0)$ in the first spiral corresponding to $Nx < 1$. The leading behaviour of the higher-order sum for $N \to \infty$, $0 < x < 1$ and integer values of $p \geq 3$ was obtained in [3; 10, §3.7]. Coutsias & Kazarinoff [4] derived an expansion for $S_N(x, 0)$ valid as $x \to 0$ and finite Nx although, as they were principally concerned with improving the order estimate in (1.2), one of their terms was left as an order estimate. Their procedure was to employ the Poisson summation formula in the form

$$S_N(x,0) = \sum_{k=-\infty}^{\infty} \int_{-N}^{N} \exp\{2\pi i\phi_k(t)\}dt,$$

where $\phi_k(t) = \frac{1}{2}xt^2 + kt$, and decompose the resulting sum according to where the stationary point (given by $\phi_k' = 0$) of the phase of the kth term is situated with respect to the interval $(-N, N)$.

In this paper, we derive the expansion of $S_N(x,\theta)$ as $x \to 0$ and $N \to \infty$ such that $Nx = O(1)$ in the case $\theta \neq 0$ by a more direct method using the Abel-Plana form of the Euler-Maclaurin summation formula. The sum $S_N(x,\theta)$ is expressed exactly as a series of complementary error functions with argument proportional to $x^{-1/2}$. The resulting expansion of $S_N(x,\theta)$ as $x \to 0$ then follows from the asymptotics of the complementary error function. The expansion so obtained breaks down in the neighbourhood of integer values of $Nx + \theta$; we describe the modification required to produce an expansion that remains valid uniformly in $Nx+\theta$. Numerical results are given to demonstrate the accuracy of the different expansions.

Finally, the generalised Gauss sum (1.1) can be extended by changing the exponential factor to $\exp\{\pi i x p_k(j)\}$, where $p_k(z)$ is a polynomial in z of degree k such that $p_k'(z) \geq 0$ and $p_k''(z) \geq 0$ for $z \geq 0$. A leading order estimate of this generalised exponential sum (a Weyl sum) when x is small has been obtained in [11]. A related, though quite different, asymptotic problem with $p_k(z) = z^k$, $x = ia$ $(a > 0)$ and $N = \infty$ (the so-called Euler-Jacobi sum) has been considered in the limit $a \to 0$ in [9] for integer k and in [16, §8.1] for $k > 1$. The expansion of the sum in this case is found to consist of an algebraic expansion together with a sequence of exponentially small expansions whose number increases by one — manifested by means of a Stokes phenomenon — each time k passes through the values 2(mod 4).

2. The expansion of $S_N(x,\theta)$ for $x \to 0$

Let N be a positive integer, $0 < x < 1$, $-\frac{1}{2} \leq \theta \leq \frac{1}{2}$ and define the quantity $\xi := Nx + \theta$. Then, with $f(t) = \exp(\pi i x t^2 + 2\pi i\theta t)$, we have by Cauchy's theorem

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

where $\mathcal{C}$ is a closed path encircling only the poles of the integrand at $t = 1, 2, \ldots, N-1$. Following (with a slight modification) the derivation of the Abel-Plana form of the Euler-Maclaurin summation formula given in [14, p. 290], we deform the path $\mathcal{C}$ into the parallelogram with vertices at $\pm Pe^{\pi i/4}$, $N \pm Pe^{\pi i/4}$ $(P > 0)$ and with semi-circular indentations of radius $\delta < 1$ around the points $t = 0$ and $t = N$; see Fig. 2. Then, denoting the upper and lower

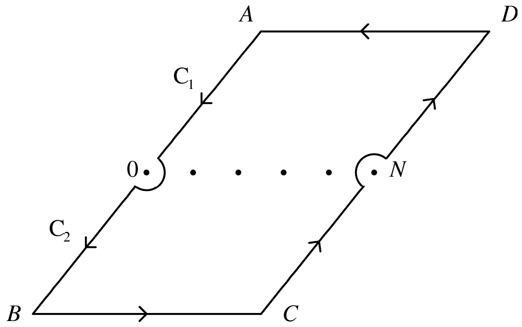

Figure 2: The contours $\mathcal{C}_1$ and $\mathcal{C}_2$ with the vertices A, B at $\pm Pe^{\pi i/4}$ and C, D at $N \mp Pe^{\pi i/4}$, respectively. The heavy dots denote the poles of the integrand.

parts of the contour by $\mathcal{C}_1$ and $\mathcal{C}_2$ respectively, we find[1] [14, p. 290]

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

Now let $P \to \infty$, so that the contributions from the parts of $\mathcal{C}_1$ and $\mathcal{C}_2$ parallel to the real axis vanish on account of the exponential decay of the factor $\exp(\pi ixt^2)$, 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 other indentation at $t = N$. Thus we obtain

$$S_N(x,\theta) = {\sum_{j=0}^{N}}' f(j) = e^{\pi i/4}(I_N - I_0) + \int_0^N f(t)\,dt, \tag{2.1}$$

where

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

with

$$F_n(\tau) := f(n-\tau e^{\pi i/4}) - f(n+\tau e^{\pi i/4}) = 2e^{-\pi x\tau^2} f(n) \sinh\{2\pi(nx+\theta)\omega\tau\},$$

and, for convenience, we have set $\omega := e^{-\pi i/4}$. The prime on the summation sign signifies that the first and last terms in the sum are halved. We remark that $F_0(\tau) \equiv 0$ when $\theta = 0$.

[1] We remark that this procedure is similar to that employed in [10, §2.2].

We now consider in turn each of the integrals appearing (2.1). In the integral I_N, we substitute the identity

$$\frac{1}{e^{2\pi\omega\tau}-1}=\sum_{k=1}^{K}e^{-2\pi k\omega\tau}+\frac{e^{-2\pi K\omega\tau}}{e^{2\pi\omega\tau}-1},$$

where K denotes an arbitrary positive integer. Then we find

$$\begin{aligned} I_N &= 2f(N)\sum_{k=1}^{K}\int_0^\infty e^{-\pi x\tau^2-2\pi k\omega\tau}\sinh(2\pi\xi\omega\tau)\,d\tau+H_K \\ &= \frac{f(N)}{\sqrt{2\pi x}}\sum_{k=1}^{K}\int_0^\infty e^{-\frac{1}{2}u^2}(e^{-uz_k^-}-e^{-uz_k^+})du+H_K, \end{aligned} \tag{2.2}$$

where $u=(2\pi x)^{1/2}\tau$ and

$$z_k^{\pm}=(2\pi/x)^{1/2}\,(k\pm\xi)\,e^{-\pi i/4}. \tag{2.3}$$

The remainder H_K is given by

$$H_K=\int_0^\infty\frac{e^{-2\pi K\omega\tau}F_N(\tau)}{e^{2\pi\omega\tau}-1}d\tau=f(N)\int_0^\infty e^{-\pi x\tau^2-(2K+1)\pi\omega\tau}G(\tau)\,d\tau,$$

with $G(\tau)=\sinh(2\pi\xi\omega\tau)/\sinh(\pi\omega\tau)$. It is easy to show that, when $0<x<1$ and $|\theta|\le\frac{1}{2}$, the quantity $|e^{-2\pi N\omega\tau}G(\tau)|$ is monotonically decreasing on $[0,\infty)$ and bounded by 2ξ. Hence, provided $K>N$,

$$|H_K|<2\xi\int_0^\infty e^{-2\pi(K-N)\mathrm{Re}(\omega)\tau}d\tau=\frac{\xi\sqrt{2}}{\pi(K-N)}$$

so that $H_K\to 0$ as $K\to\infty$. The integrals appearing on the right-hand side of (2.2) can be evaluated in terms of the complementary error function $\mathrm{erfc}\,(z)$ to obtain, with K set equal to ∞,

$$I_N=\frac{f(N)}{2\sqrt{x}}\sum_{k=1}^{\infty}E(z_k^-)-E(z_k^+), \tag{2.4}$$

where we have defined $E(z)$ by

$$E(z):=\sqrt{\frac{2}{\pi}}\int_0^\infty e^{-\frac{1}{2}u^2-zu}du=e^{\frac{1}{2}z^2}\mathrm{erfc}\,(z/\sqrt{2}). \tag{2.5}$$

We now let $x\to 0$ and set $\xi=Nx+\theta=M+\epsilon$, where $M=[\xi]$ denotes the nearest integer part of ξ and $-\frac{1}{2}<\epsilon\le\frac{1}{2}$. The values of the variable z_k^+ lie on the ray $\arg z=-\frac{1}{4}\pi$ for $k\ge 1$, while the values of z_k^- lie on the rays

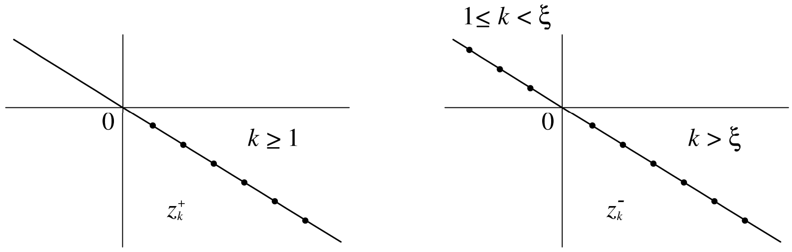

Figure 3: The points $z_k^\pm$ for $k = 1, 2, \ldots$.

$\arg z = \frac{3}{4}\pi$ when $k < \xi$ and $\arg z = -\frac{1}{4}\pi$ when $k > \xi$; see Fig. 3. Then, provided $|\epsilon| >> x^{1/2}$, it is clear that $|z_k^\pm| \to \infty$ uniformly in k as $x \to 0$. The expansion of $E(z)$ as $|z| \to \infty$ is [1, Eq. (7.1.23)]

$$E(z) = \begin{cases} \dfrac{1}{\pi}\displaystyle\sum_{r=0}^{n-1}(-)^r\,\Gamma(r+\tfrac{1}{2})(\tfrac{1}{2}z^2)^{-r-\frac{1}{2}} + R_n(z) & (|\arg z| < \tfrac{3}{4}\pi) \\ \\ 2\,e^{\frac{1}{2}z^2} + \dfrac{1}{\pi}\displaystyle\sum_{r=0}^{n-1}(-)^r\,\Gamma(r+\tfrac{1}{2})(\tfrac{1}{2}z^2)^{-r-\frac{1}{2}} - R_n(-z) & (|\arg(-z)| < \tfrac{3}{4}\pi), \end{cases} \tag{2.6}$$

where the second expansion follows from the first and the well-known reflection formula $\mathrm{erfc}\,(z) = 2 - \mathrm{erfc}\,(-z)$. The remainder $R_n(z)$ after n terms satisfies the bound[2]

$$|R_n(z)| \leq \frac{2^{n+\frac{1}{2}}}{\pi}\,\Gamma(n+\tfrac{1}{2})\,|z|^{-2n-1} \qquad (|\arg z| \leq \tfrac{1}{4}\pi). \tag{2.7}$$

Substitution of the expansions (2.6a) (with $z = z_k^+$ (for $k \geq 1$) and $z = z_k^-$ (for $k > \xi$)) and (2.6b) (with $z = z_k^-$ (for $k < \xi$)) into (2.4) then yields after a little algebraic simplification

$$\begin{aligned} I_N \;=\; & \frac{1}{2}f(N)\sum_{r=0}^{n-1}(-)^{r-1}\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}(\pi i x)^r c_r(\xi) \\ & \qquad + \frac{f(N)}{\sqrt{x}}\sum_{k<\xi} e^{-\pi i(k-\xi)^2/x} + \mathcal{R}_n(x;\xi) \end{aligned} \tag{2.8}$$

for $n = 1, 2, \ldots$. The coefficients $c_r(\xi)$ are given by

$$c_r(\xi) = \frac{1}{\pi^{2r+1}}\sum_{\substack{k=-\infty \\ k\neq 0}}^{\infty}(k+\xi)^{-2r-1}, \tag{2.9}$$

[2] This follows from the relation $\Gamma(\frac{1}{2}, z^2) = \sqrt{\pi}\,\mathrm{erfc}\,(z)$ connecting the complementary error function to the incomplete gamma function and the error bound for $\Gamma(a, z)$ given in [14, p. 111].

where the sum corresponding to $r = 0$ must be interpreted in the principal value sense $\sum_{k=-\infty}^{\infty} a_k = \lim_{M\to\infty} \sum_{k=-M}^{M} a_k$. The explicit representation of the first few coefficients $c_r(\xi)$ is given in §3. We observe that when $\xi < 1$ the second sum in (2.8) is empty.

The remainder term $\mathcal{R}_n(x;\xi)$ is given by

$$\mathcal{R}_n(x;\xi) = \frac{f(N)}{\sqrt{2\pi x}}\Big\{\sum_{k>\xi} R_n(z_k^-) - \sum_{k<\xi} R_n(-z_k^-) - \sum_{k\geq 1} R_n(z_k^+)\Big\}, \tag{2.10}$$

so that, by (2.3) and (2.7),

$$\begin{aligned}|\mathcal{R}_n(x;\xi)| &\leq \frac{1}{\sqrt{2\pi x}}\Big\{\sum_{k\geq 1} |R_n(z_k^+)| + \sum_{k>\xi} |R_n(z_k^-)| + \sum_{k<\xi} |R_n(-z_k^-)|\Big\} \\ &\leq \frac{2^{n-\frac{1}{2}}}{\pi^2}\,\Gamma(n+\tfrac{1}{2})\left(\frac{x}{2\pi}\right)^n A_n(\xi), \quad A_n(\xi) = \sum_{\substack{k=-\infty\\ k\neq 0}}^{\infty} |k+\xi|^{-\alpha_n} \end{aligned} \tag{2.11}$$

where $\alpha_n := 2n+1$ $(n \geq 1)$. Then, with $\xi = M + \epsilon$, where M and ϵ are as defined above, we have

$$\begin{aligned} A_n(\xi) &= \sum_{k=0}^{M-1} |k+\epsilon|^{-\alpha_n} + \sum_{k=1}^{\infty} (k-\epsilon)^{-\alpha_n} + \sum_{k=M+1}^{\infty} (k+\epsilon)^{-\alpha_n} \\ &< \frac{1}{(1-\epsilon)^{\alpha_n}} + \frac{\beta_0}{\epsilon^{\alpha_n}} + \sum_{k=1}^{\infty}(k+1-\epsilon)^{-\alpha_n} + \sum_{k=1}^{\infty}(k+\epsilon)^{-\alpha_n} \\ &< \frac{1}{(1-\epsilon)^{\alpha_n}} + \frac{\beta_0}{\epsilon^{\alpha_n}} + \frac{\beta_1}{(1+\epsilon)^{\alpha_n}} + 2\zeta(\alpha_n), \end{aligned} \tag{2.12}$$

where $\beta_r = 1 - \delta_{M,r}$ $(r = 0, 1)$, with $\delta_{M,r}$ being the Kronecker symbol, and $\zeta(\alpha_n)$ is the Riemann zeta function. Since, from (2.9), $|c_r(\xi)| < A_r(\xi)/\pi^{2r+1}$ it is readily seen that the above expansion for I_N possesses an asymptotic character for $x \to 0$ when $M = 0$, and provided $\epsilon >> x^{1/2}$ when $M \geq 1$.

For the integral involving $F_0(\tau)$ in (2.1), the variables $z_k^{\pm} = (2\pi/x)^{1/2}(k \pm \theta)e^{-\pi i/4}$ so that $|z_k^{\pm}| \to \infty$ when $x \to 0$ for $k \geq 1$. We then immediately obtain from (2.8) the asymptotic expansion

$$I_0 = \frac{1}{2}\sum_{r=0}^{n-1}(-)^{r-1}\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}(\pi i x)^r c_r(\theta) + \mathcal{R}_n(x;\theta) \tag{2.13}$$

as $x \to 0$, where $c_r(\theta)$ and $|\mathcal{R}_n(x;\theta)|$ are given by (2.9) and (2.11) (with ξ replaced by θ) and from (2.12)

$$A_n(\theta) < 1 + 2\zeta(\alpha_n) + (1 - |\theta|)^{-\alpha_n}. \tag{2.14}$$

We remark that, from (2.9), the coefficients $c_r(0) = 0$ $(r \geq 0)$.

Finally, the integral over the interval $[0, N]$ can be evaluated in terms of the error function [1, p. 297] as

$$J_N := \int_0^N f(t)\,dt \;=\; e^{-\pi i\theta^2/x}\int_0^N e^{\pi ix(t+\theta/x)^2}dt = e^{-\pi i\theta^2/x}\int_{\theta/x}^{\xi/x} e^{\pi ix\tau^2}d\tau$$
$$= \frac{e^{-\pi i\theta^2/x+\pi i/4}}{2\sqrt{x}}\Big\{\mathrm{erf}\,(\omega\xi\sqrt{\pi/x}\,) - \mathrm{erf}\,(\omega\theta\sqrt{\pi/x}\,)\Big\}. \quad (2.15)$$

Then upon noting that

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

and collecting together the results in (2.1), (2.8), (2.13) and (2.15), we obtain

Theorem 1 *Let $S_N(x, \theta)$ be the sum defined in (2.1), where $0 < x < 1$, $-\frac{1}{2} \leq \theta \leq \frac{1}{2}$, N is a positive integer and $\xi := Nx + \theta$. Then, as $x \to 0$ we have the asymptotic expansion*

$$S_N(x, \theta) \;=\; J_N + \frac{1}{2i}\sum_{r=0}^{n-1}(-)^r\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}(\pi ix)^r C_r$$
$$+\frac{e^{-\pi i\theta^2/x+\pi i/4}}{\sqrt{x}}\sum_{k<\xi} e^{-\pi ik^2/x+2\pi ik\theta/x} + \tilde{R}_n, \quad (2.16)$$

where $n = 1, 2, \ldots$ and J_N is given by (2.15). The coefficients C_r are defined by

$$C_r = f(N)c_r(\xi) - c_r(\theta), \quad (2.17)$$

where c_r are defined in (2.9) and are explicitly represented in §3. The remainder $\tilde{R}_n$

$$\tilde{R}_n = \mathcal{R}_n(x; \xi) - \mathcal{R}_n(x; \theta),$$

where $\mathcal{R}_n(x; \xi)$ and $\mathcal{R}_n(x; \theta)$ have the bounds in (2.11), (2.12) and (2.14) expressed in terms of $\epsilon = \xi - [\xi]$. The expansion (2.16) holds without restriction when $M = [\xi] = 0$ and provided $|\epsilon\,| >> x^{1/2}$ when $M \geq 1$.

When $\epsilon = o(x^{1/2})$ and $M \geq 1$ the expansion in (2.16) breaks down since, when $k = M = [\xi]$, the argument of the term $E(z_M^-)$ in (2.4) has the value

$$z_M^- = -\epsilon\,(2\pi/x)^{1/2}\,e^{-\pi i/4}$$

and so lies in a neighbourhood of the origin; see Fig. 3. Furthermore, the bound for the remainder $\mathcal{R}_n(x; \xi)$ in (2.11) and (2.12) similarly contains a term that behaves like x^n/ϵ^{2n+1} (when $M \geq 1$). In this case it is no longer meaningful to employ the asymptotic expansions in (2.6) for $E(z_k^-)$ when $k = M$. To overcome this difficulty, we simply leave this latter term in (2.4) as it is and delete the corresponding term from the coefficients $c_r(\xi)$ to produce the new (regularised) coefficients $c_r'(\xi)$ defined by

$$c_r'(\xi) = c_r(\xi) - (\pi\epsilon)^{-2r-1}. \tag{2.18}$$

Then the modified expansion for I_N in (2.8) becomes (for $M \geq 1$)

$$I_N = \frac{1}{2}f(N)\sum_{r=0}^{n-1}(-)^{r-1}\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}(\pi ix)^r c_r'(\xi) - a(\epsilon)\frac{f(N)}{2\sqrt{x}}\,E(\mp z_M^-)$$
$$+\frac{e^{-\pi i\theta^2/x}}{\sqrt{x}}\sum_{k\leq\xi}{}^{*}\, e^{-\pi ik^2/x+2\pi ik\theta/x} + \mathcal{R}_n'(x;\xi), \tag{2.19}$$

where we have employed the reflection formula for $\mathrm{erfc}\,(z)$ when $\epsilon > 0$ stated at (2.6), the upper or lower sign is chosen according as $\epsilon > 0$ or $\epsilon < 0$, respectively, and $a(\epsilon) = 1$ ($\epsilon > 0$), 0 ($\epsilon = 0$), -1 ($\epsilon < 0$). The asterisk on the summation sign signifies that when $\epsilon = 0$ ($\xi = M$) the last term in the sum is halved.[3] The prime on the remainder similarly denotes the deletion of the term corresponding to $k = M$ in (2.10), so that $\mathcal{R}_n'(x;\xi)$ satisfies the bound (2.11), but with $A_n(\xi)$ given by the bound (2.12) with the term $\epsilon^{-\alpha_n}$ deleted. Then we have

Theorem 2 *Let $S_N(x,\theta)$ be the sum defined in (2.1), where $0 < x < 1$, $-\frac{1}{2} \leq \theta \leq \frac{1}{2}$, N is a positive integer and $\xi := Nx + \theta$. Then, as $x \to 0$ we have the asymptotic expansion*

$$\begin{aligned} S_N(x,\theta) \;=\; & J_N + \frac{1}{2i}\sum_{r=0}^{n-1}(-)^r\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}(\pi ix)^r C_r' - a(\epsilon)e^{\pi i/4}\frac{f(N)}{2\sqrt{x}}\,E(\mp z_M^-) \\ & +\frac{e^{-\pi i\theta^2/x+\pi i/4}}{\sqrt{x}}\sum_{k\leq\xi}{}^{*}\, e^{-\pi ik^2/x+2\pi ik\theta/x} + \tilde{R}_n', \end{aligned} \tag{2.20}$$

where $n = 1, 2, \ldots$, $a(\epsilon) = 1$, ($\epsilon > 0$), 0 ($\epsilon = 0$), -1 ($\epsilon < 0$), J_N is given by (2.15) and $E(z)$ is defined in (2.6). The upper or lower sign is chosen according as $\epsilon > 0$ or $\epsilon < 0$, respectively. The coefficients C_r' are defined by

$$C_r' = f(N)c_r'(\xi) - c_r(\theta),$$

[3] This results from the fact that $E(0) = 1$.

where $c_r'(\xi)$ and $c_r(\theta)$ are defined in (2.18) and (2.9) and are explicitly represented in §3. The remainder $\tilde{R}_n'$

$$\tilde{R}_n' = \mathcal{R}_n'(x;\xi) - \mathcal{R}_n(x;\theta),$$

where $\mathcal{R}_n'(x;\xi)$ and $\mathcal{R}_n(x;\theta)$ have the bounds in (2.11) and (2.12) with the term $\epsilon^{-\alpha_n}$ deleted, and in (2.11) and (2.14), respectively. The expansion (2.20) holds uniformly in $\epsilon = \xi - [\xi]$ and, in particular, in the neighbourhood of $\epsilon = 0$.

3. Numerical results and discussion

We present results of numerical calculations using the expansions for $S_N(x,\theta)$ in (2.16) and (2.20) truncated after $n \le 4$ terms. The coefficients $c_r(\xi)$ (and $c_r(\theta)$) defined in (2.9), which appear in the expansion in (2.16), can be evaluated in the form

$$c_0(\xi) = \cot(\pi\xi) - \frac{1}{\pi\xi}, \qquad c_r(\xi) = \frac{1}{(2r)!}\frac{d^{2r}c_0(\xi)}{d(\pi\xi)^{2r}} \quad (r \ge 1). \tag{3.1}$$

Explicit representations for the first few coefficients with $r \ge 1$ are therefore given by

$$\begin{aligned} c_1(\xi) &= \frac{\cot(\pi\xi)}{\sin^2(\pi\xi)} - \frac{1}{(\pi\xi)^3}, \\ c_2(\xi) &= \frac{\cot(\pi\xi)}{\sin^2(\pi\xi)}\left(\frac{1}{3}\cot^2(\pi\xi) + \frac{2}{3}\frac{1}{\sin^2(\pi\xi)}\right) - \frac{1}{(\pi\xi)^5}, \\ c_3(\xi) &= \frac{\cot(\pi\xi)}{\sin^2(\pi\xi)}\left(\frac{2}{45}\cot^4(\pi\xi) + \frac{26}{45}\frac{\cot^2(\pi\xi)}{\sin^2(\pi\xi)} + \frac{17}{45}\frac{1}{\sin^4(\pi\xi)}\right) - \frac{1}{(\pi\xi)^7}, \ \ldots . \end{aligned} \tag{3.2}$$

These coefficients have a removable singularity at $\xi = 0$, as can be seen from the expansions valid for small ξ

$$c_0(\xi) = -\frac{\pi\xi}{3} - \frac{(\pi\xi)^3}{45} - \cdots, \quad c_1(\xi) = -\frac{\pi\xi}{15} - \frac{4(\pi\xi)^3}{189} - \cdots,$$

and so on, but are singular whenever ξ equals a positive integer. The regularised coefficients $c_r'(\xi)$ appearing in the expansion (2.20) become, with $\xi = M + \epsilon$ and $M = [\xi]$,

$$c_r'(\xi) := c_r(\xi) - (\pi\epsilon)^{-2r-1} = c_r(\epsilon) - (\pi\xi)^{-2r-1}, \tag{3.3}$$

which are thus seen to be regular when $\xi = M$. Computation of the coefficients $c_r'(\xi)$ then follows straightforwardly from (3.2), unless ϵ is very close to zero in which case a series expansion for $c_r(\epsilon)$ can be employed.

In Tables 1 and 2, we show the absolute value of the error in the computation of $S_N(x,\theta)$ using the expansions (2.16) and (2.20), respectively, for several values of x, θ, truncation index N and different levels n. The exact value of $S_N(x,\theta)$ was obtained by high-precision summation of (1.1). Note that in Table 2 we have chosen some values of ξ in the neighbourhood of integer values to demonstrate the accuracy of the modified expansion (2.20) in this limit. In Fig. 4 we compare the absolute value of the error in the expansions in (2.16) and (2.20) when $x=1/(250\sqrt{3})$ and $\theta=0.3$ with $n=4$ and for the truncation index N in the range $5900\leq N\leq 6400$; this corresponds to values of ξ ranging from just less than 14 to just greater than 15. It can be seen that the expansion (2.16) yields greatest accuracy when $\epsilon\simeq\frac{1}{2}$ and progressively deteriorates as ξ approaches integer values ($\epsilon\to 0$). The expansion (2.20), on the other hand, yields uniform accuracy in the neighbourhood of integer values of ξ and is least accurate (although comparable with that of (2.16)) when $\epsilon\simeq\frac{1}{2}$.

n	$x=10^{-2},\ \theta=0.40$ $N=1000,\ \xi=10.4$	$x=10^{-4},\ \theta=-0.20$ $N=5000,\ \xi=0.30$
1	3.954×10^{-3}	1.037×10^{-5}
2	1.178×10^{-4}	1.019×10^{-9}
3	5.852×10^{-6}	1.589×10^{-13}
4	4.067×10^{-7}	3.426×10^{-17}
n	$x=1/(200\sqrt{\pi}),\ \theta=0.10$ $N=9000,\ \xi\doteq 25.489$	$x=1/(250\sqrt{3}),\ \theta=0.30$ $N=6150,\ \xi\doteq 14.503$
1	5.289×10^{-5}	1.623×10^{-4}
2	6.331×10^{-7}	4.437×10^{-7}
3	8.667×10^{-9}	2.299×10^{-9}
4	1.438×10^{-10}	2.088×10^{-11}

Table 1: Values of the absolute error in the computation of $S_N(x,\theta)$ by (2.16) for different truncation index n.

Finally, in the case of the classical quadratic Gauss sum ($\theta=0$) we obtain from (2.16)

$$S_N(x,0)=\frac{e^{\pi i/4}}{2\sqrt{x}}\,\mathrm{erf}\,(e^{-\pi i/4}N\sqrt{\pi x})+\frac{f(N)}{2i}\sum_{r=0}^{n-1}(-)^r\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}(\pi ix)^r c_r(\xi)$$

n	$x=\pi/500,\ \ \theta=0.25$ $N=12000,\ \ \xi\doteq 75.648$	$x=1/(250\sqrt{\pi}),\ \ \theta=0.10$ $N=6600,\ \ \xi\doteq 14.995$
1	4.612×10^{-4}	3.901×10^{-5}
2	3.458×10^{-6}	6.834×10^{-8}
3	4.253×10^{-8}	1.781×10^{-10}
4	7.301×10^{-10}	6.099×10^{-13}
n	$x=1/(200\sqrt{3}),\ \ \theta=0.20$ $N=7552,\ \ \xi\doteq 22.001$	$x=1/(500\sqrt{3}),\ \ \theta=1/\sqrt{5}$ $N=12600,\ \ \xi\doteq 14.996$
1	1.076×10^{-4}	1.716×10^{-4}
2	2.700×10^{-7}	3.122×10^{-7}
3	1.040×10^{-9}	9.397×10^{-10}
4	5.397×10^{-12}	3.956×10^{-12}

Table 2: Values of the absolute error in the computation of $S_N(x,\theta)$ by (2.20) for different truncation index n.

$$+\frac{e^{\pi i/4}}{\sqrt{x}}\sum_{k<\xi} e^{-\pi ik^2/x}+\mathcal{R}_n(x;\xi) \tag{3.4}$$

as $x\to 0$, where $\xi=Nx$. This expansion breaks down as $\epsilon=\xi-[\xi]\to 0$ when $M\geq 1$. An expansion equivalent to this has been given in [4]. The modified version of this expansion obtained from (2.20) takes the form

$$S_N(x,0)=\frac{e^{\pi i/4}}{2\sqrt{x}}\,\mathrm{erf}\,(e^{-\pi i/4}N\sqrt{\pi x})+\frac{f(N)}{2i}\sum_{r=0}^{n-1}(-)^r\frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}(\pi ix)^r c_r'(\xi)$$

$$-a(\epsilon)\frac{f(N)}{2\sqrt{x}}e^{-\pi i\epsilon^2/x+\pi i/4}\,\mathrm{erfc}\,(e^{-\pi i/4}\epsilon\sqrt{\pi/x})$$

$$+\frac{e^{\pi i/4}}{\sqrt{x}}\sum_{k\leq\xi}{}^{*}\,e^{-\pi ik^2/x}+\mathcal{R}_n'(x;\xi), \tag{3.5}$$

which remains valid in the neighbourhood of integer values of ξ. We remark that, when $\theta=0$, the parameter ξ can only equal an integer value when x is a rational fraction; for irrational x the halving of the last term in the second sum in (3.5) can never occur. As we have seen in §1, the case of rational x for the quadratic Gauss sum is less challenging, since the trace of the terms in this case presents a 'block-symmetry'.

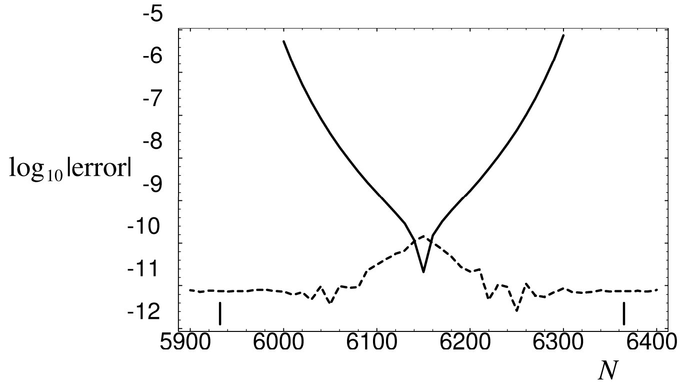

Figure 4: The absolute error (on a $\log_{10}$ scale) in the expansions (2.16) (solid curve) and (2.20) (dashed curve) as a function of N when $x = 1/(250\sqrt{3})$, $\theta = 0.3$ and $n = 4$. The small vertical marks denote the positions corresponding to $\xi = 14$ and $\xi = 15$.

Expansions of the higher-order Gauss sum $\sum_{j=0}^{N} \exp(\pi i x j^p)$ valid in the principal spiral $pxN^{p-1}/2 < 1$ have been given in [6, 15]. The expansion (3.4) agrees with that obtained in [15, §4] in the special case $p = 2$ when $Nx < 1$ (so that the second sum over k is empty). The expansion obtained in [6] when $p = 2$ and $Nx < 1$ also agrees with (3.4) when it is assumed that $N\sqrt{(\pi x)}$ is sufficiently large to justify use of the asymptotic expansion of the complementary error function. In Table 3 we display the value of the absolute error in the evaluation of $S_N(x, 0)$ by means of the regularised expansion (3.5) for different values x and N, and in particular in the neighbourhood of integer values of $\xi = Nx$.

n	$x = \pi/500,\ \ N = 4500$ $\xi \doteq 28.274$	$x = 1/400\ \ N = 5201$ $\xi = 13.0025$
1	3.623×10^{-4}	1.057×10^{-6}
2	2.256×10^{-6}	1.923×10^{-9}
3	2.214×10^{-8}	5.285×10^{-12}
4	2.977×10^{-10}	1.887×10^{-14}
n	$x = 1/(250\sqrt{\pi})\ \ N = 7100$ $\xi \doteq 16.023$	$x = 1/(500\sqrt{5})\ \ N = 1100$ $\xi \doteq 0.984$
1	8.560×10^{-6}	2.141×10^{-5}
2	1.446×10^{-8}	8.904×10^{-9}
3	3.597×10^{-11}	6.151×10^{-12}
4	1.163×10^{-13}	5.940×10^{-15}

Table 3: Values of the absolute error in the computation of $S_N(x, 0)$ by (3.5) for different truncation index n.

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