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Schlömilch series that arise in diffraction theory and their efficient computation

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Abstract

We are concerned with a certain class of Schlömilch series that arise naturally in the study of diffraction problems when the scatterer is a semi-infinite periodic structure. By combining new results derived from integral representations and the Poisson summation formula with known identities, we obtain expressions which enable the series to be computed accurately and efficiently. Many of the technical details of the derivations are omitted; they can, however, be obtained from Linton 2005 Schlömilch series that arise in diffraction theory and their efficient computation *Technical Report* Loughborough University available online at <http://www-staff.lboro.ac.uk/~macml1/schlomilch-techreport.pdf>.

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1. Introduction

A Schlömilch series is a series of the form $\sum_j a_j(x) Z_n(jx)$, where $Z_n(\cdot)$ is a Bessel function. A general discussion of such series can be found in [2, chapter XIX] and they continue to be the subject of research (see [3, 4] for example). We are concerned here with the series

$$S_n^\pm(x, \beta) = \sum_{j=1}^{\infty} H_n(jx) e^{\pm ij\beta x}, \quad x > 0, \quad 0 \leq \beta \leq \pi/x, \quad (1)$$

where $H_n(\cdot) \equiv H_n^{(1)}(\cdot)$ is a Hankel function of the first kind, and others which are related to them. We will assume that $n \geq 0$; results for negative n can then be obtained from $S_{-n}^\pm = (-1)^n S_n^\pm$. Clearly $S_n^\pm(x, \beta)$ is a periodic function of β with period $2\pi/x$, but

$$S_n^\pm(x, 2\pi/x - \beta) = S_n^\mp(x, \beta) \quad (2)$$

and so it suffices to consider only the range $0 \leq \beta \leq \pi/x$. The sums S_n^\pm can then be evaluated for all β by first reducing β to the interval $[0, 2\pi/x)$ using periodicity and then using (2) if necessary.

Related to S_n^\pm are the series (often referred to as lattice sums)

$$\sigma_n = \sum_{j=1}^{\infty} H_n(jx)[(-1)^n e^{ij\beta x} + e^{-ij\beta x}] = (-1)^n S_n^+ + S_n^- \quad (3)$$

which arise naturally in diffraction problems where the scatterer is an infinite periodic structure. In the form given above, they are totally unsuitable for numerical evaluation, but Twersky [5] showed how these series can be transformed into new expressions which are amenable to computation. An alternative approach, using recurrence relations, is described in [6].

When it comes to semi-infinite arrays, however, it is the series S_n^\pm that are fundamental and it is the objective of this paper to derive expressions which enable these sums to be computed efficiently. It will be convenient to work also with the related series

$$\mathcal{J}_n^c = \sum_{j=1}^{\infty} J_n(jx) \cos j\beta x, \quad \mathcal{Y}_n^c = \sum_{j=1}^{\infty} Y_n(jx) \cos j\beta x, \quad (4)$$

$$\mathcal{J}_n^s = \sum_{j=1}^{\infty} J_n(jx) \sin j\beta x, \quad \mathcal{Y}_n^s = \sum_{j=1}^{\infty} Y_n(jx) \sin j\beta x, \quad (5)$$

from which S_n^\pm can be constructed via

$$S_n^\pm = \mathcal{J}_n^c \mp \mathcal{Y}_n^s + i(\mathcal{Y}_n^c \pm \mathcal{J}_n^s). \quad (6)$$

In the diffraction context, the series σ_n can be thought of as the effect at the origin due to an infinite array of singularities periodically spaced along a line through the origin (spacing governed by the parameter x) with a constant phase difference (governed by the parameter β). The key to the efficient computation of σ_n (and of S_n^\pm) is to transform the representation into a sum over 'plane waves' and in order to do this we introduce the quantities (often referred to as scattering angles) ψ_m , $m \in \mathbb{Z}$ (\mathbb{Z} is the set of all integers $\{0, \pm 1, \pm 2, \dots\}$), defined by

$$\cos \psi_m = \beta_m, \quad \beta_m = \beta + 2m\pi/x. \quad (7)$$

If $|\beta_m| < 1$, we will say that $m \in \mathcal{M}$ and then $0 < \psi_m < \pi$ and $\sin \psi_m = \sqrt{1 - \beta_m^2} > 0$. If $|\beta_m| > 1$, then we will say that $m \in \mathcal{N}$, ψ_m is no longer real and the appropriate branch of the arccos function is

$$\arccos t = \begin{cases} i \operatorname{arccosh} t & t > 1 \\ \pi - i \operatorname{arccosh}(-t) & t < -1, \end{cases} \quad (8)$$

with $\operatorname{arccosh} t = \ln(t + \sqrt{t^2 - 1})$ for $t > 1$. In this case it is convenient to define $q_m > 0$ by

$$\cosh q_m = |\beta_m|, \quad \sinh q_m = \sqrt{\beta_m^2 - 1} \quad (9)$$

and then

$$\psi_m = \begin{cases} iq_m & \beta_m > 1 \\ \pi - iq_m & \beta_m < -1. \end{cases} \quad (10)$$

In either case $\sin \psi_m = i \sinh q_m$. As $|m| \rightarrow \infty$,

$$q_m \sim \ln \frac{4|m|\pi}{x} + \frac{\beta x}{2\pi m} + O(m^{-2}) \quad (11)$$

$$\sinh q_m \sim \frac{2|m|\pi}{x} + \operatorname{sgn}(m)\beta + O(m^{-1}). \quad (12)$$

Note that the set \mathcal{M} is finite and

- if $0 \leq \beta < 1$ then $0 \in \mathcal{M}$,
- if $1 < \beta \leq \pi/x$ (which can only happen if $x < \pi$) then \mathcal{M} is empty.

We will distinguish these cases by simply writing $\beta < 1$ and $\beta > 1$, respectively. Also note that if $m \geq 0$ then $\beta_m \geq 0$ and if $m < 0$ then $\beta_m < 0$.

For large j the terms in the sum in (1) have the asymptotic form (ignoring multiplicative factors) $j^{-1/2} \exp(ijx(1 \pm \beta))$. Hence, if $\beta_m = 1$ (i.e., $\psi_m = 0$) for any m then S_n^- does not exist, whereas if $\beta_m = -1$ (i.e., $\psi_m = \pi$) for any m then S_n^+ does not exist. It follows that if $|\beta_m| = 1$ for any m , the series $\sigma_n, \mathcal{J}_n^c, \mathcal{J}_n^s, \mathcal{Y}_n^c, \mathcal{Y}_n^s$ generally do not exist. It is, however, possible for both S_n^+ and S_n^- to be singular, but their singular parts cancel. Thus, for example, with $\beta = 0$ and $x = 2\pi$ (so that $\beta_{-1} = -1$ and $\beta_1 = 1$) the series \mathcal{J}_n^s and \mathcal{Y}_n^s both exist and are identically zero. Here we assume in what follows that $|\beta_m| \neq 1$ for any m (which in particular rules out the case $\beta = 1$). In the final expressions for S_n^+ (S_n^-) the value when $\beta_m = 1$ ($\beta_m = -1$) can be obtained by taking an appropriate limit.

Finally, we note that when $\beta = 0$ (which corresponds in diffraction problems to normally incident waves) we have all of the following:

$$\begin{aligned} \beta_{-m} &= -\beta_m, & \psi_{-m} &= \pi - \psi_m, & \cos \psi_{-m} &= -\cos \psi_m, \\ \sin \psi_{-m} &= \sin \psi_m, & q_{-m} &= q_m, & \psi_0 &= \pi/2, \\ S_n^+ &= S_n^-, & m \in \mathcal{M} &\Leftrightarrow -m \in \mathcal{M} \end{aligned} \quad (13)$$

and when $\beta = \pi/x$,

$$\begin{aligned} \beta_{-m} &= -\beta_{m-1}, & \psi_{-m} &= \pi - \psi_{m-1}, & \cos \psi_{-m} &= -\cos \psi_{m-1}, \\ \sin \psi_{-m} &= \sin \psi_{m-1}, & q_{-m} &= q_{m-1}, & S_n^+ &= S_n^-, \\ m \in \mathcal{M} &\Leftrightarrow -m - 1 \in \mathcal{M}. \end{aligned} \quad (14)$$

The paper is organized as follows. In section 2 we will treat the case $n = 0$. This is largely a case of gathering together formulae which already exist in the literature, though the resulting expressions for S_0^\pm appear to be new. In section 3 we give Twersky's expressions for $\sigma_n, n > 0$, and then in section 4 we show how suitable expressions can be found for all the series \mathcal{J}_n^c and \mathcal{J}_n^s . In section 5, we derive integral representations for S_n^\pm which lead to new expressions for the series defined in (4) and (5) and then in section 6 we combine the most useful representations from the different methods together to present compact and computationally efficient formulae for all the sums $S_n^\pm, n > 0$. Finally, in section 7 we make connections between the Schlömlich series under discussion here and so-called channel multipoles.

We will make extensive use of the Poisson summation formula

$$\sum_{m \in \mathbb{Z}} \int_{-\infty}^{\infty} f(u) e^{-imu} du = 2\pi \sum_{m \in \mathbb{Z}} f(2m\pi) \quad (15)$$

and use the convention that a dash on a summation sign indicates that the zeroth term is to be omitted.

2. The case $n = 0$

We will begin by deriving an exponentially convergent representation for σ_0 , both for its intrinsic interest and because it leads to a representation in terms of scattering angles which is

a first step towards computationally efficient representations for S_0^\pm . The method follows that described for a related sum in [7] and is implicit in [8]. Thus

$$\sigma_0 = \sum'_{j \in \mathbb{Z}} H_0(|j|x) e^{ij\beta x} = -\frac{i}{\pi} \sum'_{j \in \mathbb{Z}} e^{ij\beta x} \int_0^\infty \exp\left[\frac{i|j|}{2} \left(t + \frac{x^2}{t}\right)\right] \frac{dt}{t}, \quad (16)$$

[9, 8.421(8)]. Next we make the substitution $u = (t/2|j|)^{1/2} \exp(-i\pi/4)$ and deform the resulting contour from zero to infinity along the line $\arg u = -\pi/4$ into two parts: a part Γ_1 which emerges from the origin along $\arg u = -\pi/4$ and goes to the point a on the real axis (a being an arbitrary positive parameter) and then a part Γ_2 which goes from a to infinity along the real axis.

Then

$$\sigma_{\Gamma_2} = -\frac{2i}{\pi} \sum'_{j \in \mathbb{Z}} e^{ij\beta x} \int_a^\infty e^{-j^2 u^2 + x^2/4u^2} \frac{du}{u} \quad (17)$$

$$= -\frac{i}{\pi} \sum'_{j \in \mathbb{Z}} e^{ij\beta x} \sum_{n=0}^\infty \frac{1}{n!} \left(\frac{x}{2a}\right)^{2n} E_{n+1}(j^2 a^2) \quad (18)$$

in terms of the exponential integral $E_n(\cdot)$. The second expression is obtained from the first by expanding $\exp(x^2/4u^2)$ as a power series and then integrating term by term. Since $E_n(z) \sim \exp(-z)/z$, it is clear that this representation for σ_{Γ_2} is exponentially convergent in j with terms decaying like $\exp(-j^2 a^2)/j^2$ as $|j| \rightarrow \infty$.

For σ_{Γ_1} , we first note that

$$\sigma_{\Gamma_1} = -\frac{2i}{\pi} \sum'_{j \in \mathbb{Z}} e^{ij\beta x} \int_{\Gamma_1} e^{-j^2 u^2 + x^2/4u^2} \frac{du}{u} - 1 - \frac{i}{\pi} \text{Ei}(x^2/4a^2), \quad (19)$$

in terms of the exponential integral $\text{Ei}(\cdot)$. For the first term in (19), we utilize the Poisson summation formula which has the effect of transforming a series which is rapidly convergent for large u into one which is rapidly convergent for small u . Thus

$$\sigma_{\Gamma_1} = -\frac{2i}{\pi^{1/2}} \sum_{m \in \mathbb{Z}} \int_{1/a}^\infty \exp(-i\pi/4) e^{(1-\beta_m^2)x^2 s^2/4} ds - 1 - \frac{i}{\pi} \text{Ei}(x^2/4a^2). \quad (20)$$

If $(1 - \beta_m^2) < 0$, we can deform the contour back to the real axis and then the resulting integral is just a complementary error function. If $(1 - \beta_m^2) > 0$, we make the substitution $s = it$ and then the resulting contour can again be deformed back to the real axis. In either case we find that

$$\sigma_{\Gamma_1} = \frac{2}{x} \sum_{m \in \mathbb{Z}} \frac{1}{\sin \psi_m} \text{erfc}\left(-\frac{ix}{2a} \sin \psi_m\right) - 1 - \frac{i}{\pi} \text{Ei}(x^2/4a^2). \quad (21)$$

The sum over m is exponentially convergent with terms decaying like $\exp(-m^2 \pi^2/a^2)/m^2$.

Clearly increasing a speeds up the convergence of σ_{Γ_2} at the expense of σ_{Γ_1} , while decreasing a has the opposite effect. The rates of convergence of the two sums balance if we take $a = \pi^{1/2}$. In fact, series of this type serve as an excellent basis for numerical calculations (provided efficient algorithms are available for the needed special functions) and the overall computational effort is not particularly sensitive to the value of a used; see, for example, [7, 8].

If we let a tend to zero then we simply recover the Hankel function series we started with. If, however, we let a tend to infinity then $\sigma_{\Gamma_2} \rightarrow 0$ and it can be shown (using Mellin

transforms as in [4, appendix B]) that

$$\sigma_0 = S_0^- + S_0^+ = -1 - \frac{2i}{\pi} \left(C + \ln \frac{x}{4\pi} \right) + \frac{2}{x \sin \psi_0} + \sum'_{m \in \mathbb{Z}} \left(\frac{2}{x \sin \psi_m} + \frac{i}{\pi |m|} \right), \quad (22)$$

where $C \approx 0.5772$ is Euler's constant. The real part of this is

$$\mathcal{J}_0^c = -\frac{1}{2} + \sum_{m \in \mathcal{M}} \frac{1}{x \sin \psi_m} \quad (23)$$

which expresses the results of [9, 8.522(1), 8.524(1)] in compact form. If $\beta > 1$, we get $\mathcal{J}_0^c = -\frac{1}{2}$, and [9, 8.521(2)] is a special case of this with $\beta = \pi/x$. The imaginary part of (22) is

$$\mathcal{Y}_0^c = -\frac{1}{\pi} \left(C + \ln \frac{x}{4\pi} \right) - \sum_{m \in \mathcal{N}} \left(\frac{1}{x \sinh q_m} - \frac{1}{2\pi |m|} \right) + \sum'_{m \in \mathcal{M}} \frac{1}{2\pi |m|} \quad (24)$$

provided $\beta < 1$. If $\beta > 1$, then

$$\mathcal{Y}_0^c = -\frac{1}{\pi} \left(C + \ln \frac{x}{4\pi} \right) - \frac{1}{x \sinh q_0} - \sum'_{m \in \mathbb{Z}} \left(\frac{1}{x \sinh q_m} - \frac{1}{2\pi |m|} \right). \quad (25)$$

These expressions are equivalent to [9, 8.522(3), 8.524(3)].

Next, following a method similar to that outlined in [10, appendix C],

$$S_0^- - S_0^+ = \frac{1}{2} \sum_{j \in \mathbb{Z}} (e^{-i|j|\beta x} - e^{i|j|\beta x}) H_0(|j|x) = \frac{1}{2} \sum_{j \in \mathbb{Z}} f(2j\pi), \quad (26)$$

where

$$f(u) = (e^{-i|u|\beta x/2\pi} - e^{i|u|\beta x/2\pi}) H_0(|u|x/2\pi). \quad (27)$$

The Poisson summation formula (15) then leads to

$$S_0^- - S_0^+ = -\frac{2i}{x} \left(\int_0^\infty H_0(v) \sin v\beta_0 dv + \sum_{m=1}^\infty \int_0^\infty H_0(v) (\sin v\beta_m + \sin v\beta_{-m}) dv \right) \quad (28)$$

$$= \frac{4}{\pi x} \left(\frac{\frac{\pi}{2} - \psi}{\sin \psi} + \sum_{m=1}^\infty \left[\frac{\frac{\pi}{2} - \psi_m}{\sin \psi_m} + \frac{\frac{\pi}{2} - \psi_{-m}}{\sin \psi_{-m}} \right] \right), \quad (29)$$

where we have used [9, 6.671(7), (11)] which together imply that

$$\int_0^\infty H_0(v) \sin v\beta_m dv = \frac{i(1 - 2\psi_m/\pi)}{\sin \psi_m}. \quad (30)$$

Note that the sum $\sum_{m=1}^\infty \int_0^\infty H_0(v) \sin v\beta_m dv$ does not exist, but it follows from (11) and (12) that we can write

$$S_0^- - S_0^+ = \frac{4}{\pi x} \left(\frac{\frac{\pi}{2} - \psi_0}{\sin \psi_0} + \sum'_{m \in \mathbb{Z}} \left[\frac{\frac{\pi}{2} - \psi_m}{\sin \psi_m} + \frac{x i}{4m} + \frac{x}{2m\pi} \ln \frac{4|m|\pi}{x} \right] \right). \quad (31)$$

First we will assume that $\beta < 1$. Then we find that

$$\mathcal{J}_0^s = -\sum'_{m \in \mathcal{M}} \frac{1}{2m\pi} + \sum_{m \in \mathcal{N}} \left[\frac{\text{sgn}(m)}{x \sinh q_m} - \frac{1}{2m\pi} \right], \quad (32)$$

which is [9, 8.522(2)], and

$$\mathcal{Y}_0^s = \frac{2}{\pi x} \left(\frac{\frac{\pi}{2} - \psi_0}{\sin \psi_0} + \sum'_{m \in \mathcal{M}} \left[\frac{\frac{\pi}{2} - \psi_m}{\sin \psi_m} + \frac{x}{2m\pi} \ln \frac{4|m|\pi}{x} \right] - \sum_{m \in \mathcal{N}} \left[\frac{\operatorname{sgn}(m)q_m}{\sinh q_m} - \frac{x}{2m\pi} \ln \frac{4|m|\pi}{x} \right] \right). \quad (33)$$

Using (13) we can show that when $\beta = 0$, $\mathcal{J}_0^s = \mathcal{Y}_0^s = 0$ as expected. If $\beta > 1$, we have

$$\mathcal{J}_0^s = \frac{1}{x \sinh q_0} + \sum'_{m \in \mathbb{Z}} \left[\frac{\operatorname{sgn}(m)}{x \sinh q_m} - \frac{1}{2m\pi} \right], \quad (34)$$

which is [9, 8.524(2)], and

$$\mathcal{Y}_0^s = \frac{2}{\pi x} \left(\frac{-q_0}{\sinh q_0} - \sum'_{m \in \mathbb{Z}} \left[\frac{\operatorname{sgn}(m)q_m}{\sinh q_m} - \frac{x}{2m\pi} \ln \frac{4|m|\pi}{x} \right] \right). \quad (35)$$

From (22) and (31), we obtain

$$S_0^+ = -\frac{1}{2} - \frac{i}{\pi} \left(C + \ln \frac{x}{4\pi} \right) + \frac{2\psi_0/\pi}{x \sin \psi_0} + \sum'_{m \in \mathbb{Z}} \left(\frac{2\psi_m/\pi}{x \sin \psi_m} + \frac{i}{2\pi|m|} - \frac{i}{2m\pi} - \frac{1}{m\pi^2} \ln \frac{4|m|\pi}{x} \right) \quad (36)$$

and

$$S_0^- = -\frac{1}{2} - \frac{i}{\pi} \left(C + \ln \frac{x}{4\pi} \right) + \frac{2(1 - \psi_0/\pi)}{x \sin \psi_0} + \sum'_{m \in \mathbb{Z}} \left(\frac{2(1 - \psi_m/\pi)}{x \sin \psi_m} + \frac{i}{2\pi|m|} + \frac{i}{2m\pi} + \frac{1}{m\pi^2} \ln \frac{4|m|\pi}{x} \right), \quad (37)$$

the former clearly showing the singularities when $\psi_m = \pi$ and the latter when $\psi_m = 0$. The terms in the series are $O(m^{-2} \ln |m|)$ for large $|m|$, but can be accelerated if necessary. Thus, for example, we can write the sum over positive m in (36) as

$$\sum_{m=1}^{\infty} \left(\frac{2\psi_m/\pi}{x \sin \psi_m} - \frac{1}{m\pi^2} \ln \frac{4m\pi}{x} - \frac{\beta x}{2m^2\pi^3} \left[1 - \ln \frac{4m\pi}{x} \right] \right) + \frac{\beta x}{2\pi^3} \left(\frac{\pi^2}{6} \left[1 - \ln \frac{4\pi}{x} \right] + \zeta'(2) \right) \quad (38)$$

and so on, where $\zeta(\cdot)$ is the Riemann zeta function and $\zeta'(2) \approx -0.937548$.

If $\psi_p = 0$ ($\beta_p = 1$) for a particular p then S_0^+ exists and its value is easily obtained from (36) by replacing $2\psi_p/(\pi x \sin \psi_p)$ by $2/\pi x$. Similarly if $\psi_p = \pi$ ($\beta_p = -1$) for a particular p then S_0^- exists and its value is easily obtained from (37) by replacing $2(1 - \psi_p/\pi)/(x \sin \psi_p)$ by $2/\pi x$.

When $\beta = 0$ or π/x various simplifications can be made to the above expressions for \mathcal{J}_n^c etc because terms for positive and negative m combine. We will not list all these formulae here, but simply note that in either case (36) and (37) simplify to

$$S_0^+ = S_0^- = -\frac{1}{2} - \frac{i}{\pi} \left(C + \ln \frac{x}{4\pi} \right) + \frac{1}{x \sin \psi_0} + \sum'_{m \in \mathbb{Z}} \left(\frac{1}{x \sin \psi_m} + \frac{i}{2\pi|m|} \right) \quad (39)$$

the sum being divergent when $\psi_m = 0$ or π . When $\beta = 0$, we can simplify this further using (13) to

$$S_0^+ = S_0^- = -\frac{1}{2} - \frac{i}{\pi} \left(C + \ln \frac{x}{4\pi} \right) + \frac{1}{x} + \sum_{m=1}^{\infty} \left(\frac{2}{x \sin \psi_m} + \frac{i}{m\pi} \right), \quad (40)$$

whereas when $\beta = \pi/x$, (14) shows that

$$S_0^+ = S_0^- = -\frac{1}{2} - \frac{i}{\pi} \left(C - \frac{1}{2} + \ln \frac{x}{4\pi} \right) + \frac{2}{x \sin \psi_0} + \sum_{m=1}^{\infty} \left(\frac{2}{x \sin \psi_m} + \frac{i}{2m\pi} + \frac{i}{2(m+1)\pi} \right). \quad (41)$$

3. The sum σ_n for $n > 0$

Twersky [5] showed that, with the convention that $\text{sgn}(0) = +1$, we have, for $n > 0$,

$$\sigma_{2n} = 2(-1)^n \sum_{m \in \mathbb{Z}} \frac{e^{2in \text{sgn}(m)\psi_m}}{x \sin \psi_m} + 2i\lambda_{2n}, \quad (42)$$

$$\sigma_{2n-1} = 2(-1)^n i \sum_{m \in \mathbb{Z}} \frac{e^{i(2n-1)\text{sgn}(m)\psi_m}}{x \sin \psi_m} + 2\lambda_{2n-1}, \quad (43)$$

where

$$\lambda_{2n} = \frac{1}{2\pi} \sum_{m=0}^n \frac{(-1)^m 2^{2m} (n+m-1)!}{(2m)!(n-m)!} \left(\frac{2\pi}{x} \right)^{2m} B_{2m}(\beta x/2\pi), \quad (44)$$

and

$$\lambda_{2n-1} = \frac{1}{\pi} \sum_{m=0}^{n-1} \frac{(-1)^m 2^{2m} (n+m-1)!}{(2m+1)!(n-m-1)!} \left(\frac{2\pi}{x} \right)^{2m+1} B_{2m+1}(\beta x/2\pi). \quad (45)$$

Here $B_m(\cdot)$ is the Bernoulli polynomial (a finite sum; see [9, 9.620]). Note that $B_{2m+1}(0) = 0$ for $m > 0$ and $B_1(0) = -1/2$. Hence when $\beta = 0$, $\lambda_{2n-1} = -1/x$. Also $B_{2m+1}(1/2) = 0$ and so $\lambda_{2n-1} = 0$ when $\beta = \pi/x$.

The real and imaginary parts of (42) and (43) correspond to

$$\mathcal{J}_{2n}^c = (-1)^n \sum_{m \in \mathcal{M}} \frac{\cos 2n\psi_m}{x \sin \psi_m}, \quad (46)$$

$$\mathcal{Y}_{2n}^c = (-1)^n \left(\sum_{m \in \mathcal{M}} \text{sgn}(m) \frac{\sin 2n\psi_m}{x \sin \psi_m} - \sum_{m \in \mathcal{N}} \frac{e^{-2nq_m}}{x \sinh q_m} \right) + \lambda_{2n}, \quad (47)$$

$$\mathcal{J}_{2n-1}^s = -(-1)^n \sum_{m \in \mathcal{M}} \frac{\cos(2n-1)\psi_m}{x \sin \psi_m}, \quad (48)$$

$$\mathcal{Y}_{2n-1}^s = -(-1)^n \left(\sum_{m \in \mathcal{M}} \text{sgn}(m) \frac{\sin(2n-1)\psi_m}{x \sin \psi_m} - \sum_{m \in \mathcal{N}} \text{sgn}(m) \frac{e^{-(2n-1)q_m}}{x \sinh q_m} \right) + \lambda_{2n-1}. \quad (49)$$

All the infinite summations can be easily accelerated if necessary; see [7].

4. \mathcal{J}_n^c and \mathcal{J}_n^s

Computationally efficient series representations for \mathcal{J}_n^c and \mathcal{J}_n^s can be derived using methods similar to those used to derive expression (29). Thus

$$2\mathcal{J}_n^c = -J_n(0) + \sum_{j \in \mathbb{Z}} J_n(|j|x) e^{ij\beta x} \quad (50)$$

$$= -\delta_{n0} + \frac{2}{x} \sum_{m \in \mathbb{Z}} \int_0^\infty J_n(v) \cos(v\beta_m) dv, \quad (51)$$

in which we have made use of the Poisson summation formula (15). Using [9, 6.671(2)], we then get

$$\mathcal{J}_{2n}^c = -\frac{1}{2}\delta_{n0} + (-1)^n \sum_{m \in \mathcal{M}} \frac{\cos 2n\psi_m}{x \sin \psi_m} \quad (52)$$

in agreement with (23) and (46), and

$$\mathcal{J}_{2n-1}^c = -(-1)^n \sum_{m \in \mathcal{M}} \frac{\sin(2n-1)\psi_m}{x \sin \psi_m} + (-1)^n \sum_{m \in \mathcal{N}} \frac{e^{-(2n-1)q_m}}{x \sinh q_m}, \quad (53)$$

which is new. Similarly, for $n > 0$,

$$2i\mathcal{J}_n^s = \frac{1}{2} \sum_{j \in \mathbb{Z}} J_n(|j|x) (e^{ij\beta x} - e^{-ij\beta x}) \quad (54)$$

$$= \frac{i}{x} \sum_{m \in \mathbb{Z}} \int_0^\infty J_n(v) (\sin v\beta_{-m} + \sin v\beta_m) dv = \frac{2i}{x} \sum_{m \in \mathbb{Z}} \int_0^\infty J_n(v) \sin v\beta_m dv. \quad (55)$$

Note that the last step is not possible if $n = 0$, since the sum $\sum_m J_0(v) \sin v\beta_m$ does not exist. Using [9, 6.671(1)], we obtain

$$\mathcal{J}_{2n-1}^s = -(-1)^n \sum_{m \in \mathcal{M}} \frac{\cos(2n-1)\psi_m}{x \sin \psi_m} \quad (56)$$

in agreement with (48), and

$$\mathcal{J}_{2n}^s = -(-1)^n \sum_{m \in \mathcal{M}} \frac{\sin 2n\psi_m}{x \sin \psi_m} + (-1)^n \sum_{m \in \mathcal{N}} \operatorname{sgn}(m) \frac{e^{-2nq_m}}{x \sinh q_m}, \quad (57)$$

which is new.

Note that the method described in this section does not work for the sums \mathcal{Y}_n^c ($n > 0$) or \mathcal{Y}_n^s ($n > 1$) because the singularity in $Y_n(x)$ as $x \rightarrow 0$ is too strong and so the sums that arise in place of (50) and (54) cannot sensibly be defined for $j = 0$.

5. Integral representations for S_n^\pm

It is clear that when $\beta = 0$, $S_n^+ = S_n^-$. However, when $\beta \neq 0$ the manipulation of the integrals that appear below is complicated by the coalescence of a pole and a branch point. For convenience we will assume in this section that $\beta \neq 0$ and then treat the case $\beta = 0$ as part of the following section by taking the appropriate limit.

Expressions for S_n^\pm can be obtained by inserting the integral representation

$$H_n(jx) = -\frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-jx\gamma(z)}}{\gamma(z)} e^{-in \arccos z} dz, \quad (58)$$

in which $\gamma(z)$ is defined for real z by

$$\gamma(z) = \begin{cases} -i\sqrt{1-z^2} & |z| \leq 1 \\ \sqrt{z^2-1} & |z| > 1, \end{cases} \quad (59)$$

into (1) and using the generalized-function half-range summation formula (see [10])

$$\sum_{m=0}^{\infty} e^{\pm imu} = \frac{1}{1 - e^{\pm iu}} + \pi \sum_{m \in \mathbb{Z}} \delta(u + 2m\pi).$$

Thus

$$S_n^\pm = -\frac{i}{\pi} \sum_{m=0}^{\infty} e^{\pm i(m+1)\beta x} \int_{-\infty}^{\infty} \frac{e^{-(m+1)x\gamma(z)}}{\gamma(z)} e^{-in \arccos z} dz \quad (60)$$

$$\begin{aligned} &= -\frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-in \arccos z}}{\gamma(z)(e^{x\gamma(z)} \mp i\beta x - 1)} dz - i e^{\pm i\beta x} \int_{-\infty}^{\infty} \frac{e^{-x\gamma(z)}}{\gamma(z)} e^{-in \arccos z} \\ &\quad \times \sum_{m \in \mathbb{Z}} \delta(\beta_m x \pm ix\gamma(z)) dz, \end{aligned} \quad (61)$$

the integrals being interpreted as principal-value integrals where necessary. Next we use the result (see [11, p 14]) that if $g(z)$ has real simple zeros z_n , then

$$\delta(g(z)) = \sum_n \frac{\delta(z - z_n)}{|g'(z_n)|}. \quad (62)$$

In our case we have $g_\pm(z) = \beta_m x \pm ix\gamma(z)$ which has zeros when $\gamma(z) = \pm i\beta_m$. We find that

$$S_n^\pm = -\frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-in \arccos z}}{\gamma(z)(e^{x\gamma(z)} \mp i\beta x - 1)} dz + 2(\pm i)^n \sum_{m \in \mathcal{M}^\mp} \frac{\cos n\psi_m}{x \sin \psi_m}, \quad (63)$$

in which we have denoted the subset of \mathcal{M} for which $m \geq 0$ by \mathcal{M}^+ and that for which $m < 0$ by \mathcal{M}^- . Alternatively, we can write

$$S_n^\pm = -\frac{i}{\pi} \int_0^\infty \frac{h_n(z)}{\gamma(z)(e^{x\gamma(z)} \mp i\beta x - 1)} dz, \quad (64)$$

where

$$h_n(z) = e^{-in \arccos z} + (-1)^n e^{in \arccos z}. \quad (65)$$

The integral representations given above are equivalent to those derived, via a different method, in [12]. In that paper the authors computed the contour integrals directly; here we follow a different course.

We define

$$f_+(z) = \frac{\cos \beta x - e^{-x\gamma(z)}}{\gamma(z)(\cosh x\gamma(z) - \cos \beta x)}, \quad f_-(z) = \frac{i \sin \beta x}{\gamma(z)(\cosh x\gamma(z) - \cos \beta x)} \quad (66)$$

so that

$$S_n^+ + S_n^- = -\frac{i}{\pi} \int_0^\infty h_n(z) f_+(z) dz + 2i^n \sum_{m \in \mathcal{M}} (-\operatorname{sgn}(m))^n \frac{\cos n\psi_m}{x \sin \psi_m} \quad (67)$$

and

$$S_n^+ - S_n^- = -\frac{i}{\pi} \int_0^\infty h_n(z) f_-(z) dz + 2i^n \sum_{m \in \mathcal{M}} (-\operatorname{sgn}(m))^{n+1} \frac{\cos n\psi_m}{x \sin \psi_m}. \quad (68)$$

To obtain formulae for \mathcal{J}^c etc, we need to take the real and imaginary parts of the above expressions. Note that for real z with $|z| > 1$, $f_+(z)$ is real whereas $f_-(z)$ is purely imaginary; and for real z with $|z| < 1$, we have, with $g(z) = (1 - z^2)^{1/2}$,

$$f_-(z) = -\frac{\sin \beta x}{g(z)(\cos[xg(z)] - \cos \beta x)} \quad (69)$$

which is real, while

$$f_+(z) = \frac{1}{g(z)} \left(-i + \frac{\sin[xg(z)]}{\cos[xg(z)] - \cos \beta x} \right). \quad (70)$$

Note also that $h_{2n}(z)$ is real for all real z whereas $h_{2n-1}(z)$ is purely imaginary if $|z| < 1$ and real if $|z| > 1$. It is desirable to get rid of the integrable singularities at $z = 1$ and this is easily accomplished by splitting the integrals at $z = 1$ and making the change of variable $z = \cos u$ or $z = \cosh u$ as appropriate. We then obtain

$$\mathcal{J}_{2n}^c = -\frac{1}{2} \delta_{n0} + (-1)^n \sum_{m \in \mathcal{M}} \frac{\cos 2n\psi_m}{x \sin \psi_m}, \quad (71)$$

in agreement with (23) and (46),

$$\mathcal{Y}_{2n}^c = -\frac{1}{\pi} \left[\int_0^{\pi/2} \frac{\sin(x \sin u) \cos 2nu}{\cos(x \sin u) - \cos \beta x} du + \int_0^\infty \frac{(\cos \beta x - e^{-x \sinh u}) \cosh(2n \cosh u)}{\cosh(x \sinh u) - \cos \beta x} du \right], \quad (72)$$

$$\mathcal{J}_{2n-1}^c = -\frac{1}{\pi} \int_0^{\pi/2} \frac{\sin(x \sin u) \sin(2n-1)u}{\cos(x \sin u) - \cos \beta x} du, \quad (73)$$

$$\begin{aligned} \mathcal{Y}_{2n-1}^c = & \frac{1}{\pi} \left[\frac{1}{2n-1} - \int_0^\infty \frac{(\cos \beta x - e^{-x \sinh u}) \sinh(2n-1)u}{\cosh(x \sinh u) - \cos \beta x} du \right] \\ & + (-1)^n \sum_{m \in \mathcal{M}} \operatorname{sgn}(m) \frac{\cos(2n-1)\psi_m}{x \sin \psi_m}, \end{aligned} \quad (74)$$

$$\mathcal{J}_{2n}^s = \frac{\sin \beta x}{\pi} \int_0^{\pi/2} \frac{\cos 2nu}{\cos(x \sin u) - \cos \beta x} du, \quad (75)$$

$$\mathcal{Y}_{2n}^s = (-1)^n \sum_{m \in \mathcal{M}} \operatorname{sgn}(m) \frac{\cos 2n\psi_m}{x \sin \psi_m} - \frac{\sin \beta x}{\pi} \int_0^\infty \frac{\cosh 2nu}{\cosh(x \sinh u) - \cos \beta x} du, \quad (76)$$

$$\mathcal{J}_{2n-1}^s = -(-1)^n \sum_{m \in \mathcal{M}} \frac{\cos(2n-1)\psi_m}{x \sin \psi_m}, \quad (77)$$

in agreement with (48), and

$$\mathcal{Y}_{2n-1}^s = -\frac{\sin \beta x}{\pi} \left[\int_0^{\pi/2} \frac{\sin(2n-1)u}{\cos(x \sin u) - \cos \beta x} du + \int_0^\infty \frac{\sinh(2n-1)u}{\cosh(x \sinh u) - \cos \beta x} du \right]. \quad (78)$$

The computation of the Cauchy principal-value integrals can be accomplished fairly easily by first subtracting off the singular parts of the integrand. However, by combining the results of sections 3–5 we can dispense with the need to compute any principal-value integrals.

6. Computationally efficient expressions for S_n^\pm , $n > 0$

We are now in a position to write computationally efficient expressions for S_n^\pm , $n > 0$, from which all the other series can be evaluated. Using (6), we combine the results of (46)–(49) for \mathcal{J}_{2n}^c , \mathcal{Y}_{2n}^c , \mathcal{J}_{2n-1}^s , \mathcal{Y}_{2n-1}^s with (53) and (57) for \mathcal{J}_{2n-1}^c and \mathcal{J}_{2n}^s and (74) and (76) for \mathcal{Y}_{2n-1}^c and \mathcal{Y}_{2n}^s . Note that (74) and (76) do not contain principal-value integrals, only exponentially convergent ones. We obtain

$$S_n^+ = 2i^n \sum_{m=-\infty}^{-1} \frac{e^{-in\psi_m}}{x \sin \psi_m} + T_n^+ \quad (79)$$

$$S_n^- = 2(-i)^n \sum_{m=0}^{\infty} \frac{e^{in\psi_m}}{x \sin \psi_m} + T_n^-, \quad (80)$$

where

$$T_{2n-1}^\pm = \mp \lambda_{2n-1} + iL_{2n-1}, \quad T_{2n}^\pm = i\lambda_{2n} \mp L_{2n}. \quad (81)$$

Here λ_n is defined in (44) and (45) and L_n is given, from (74) and (76), by

$$L_{2n-1} = \frac{1}{\pi} \left(\frac{1}{2n-1} - \int_0^\infty \frac{(\cos \beta x - e^{-x \sinh u}) \sinh(2n-1)u}{\cosh(x \sinh u) - \cos \beta x} du \right), \quad (82)$$

$$L_{2n} = -\frac{\sin \beta x}{\pi} \int_0^\infty \frac{\cosh 2nu}{\cosh(x \sinh u) - \cos \beta x} du. \quad (83)$$

These expressions are valid for $\beta \neq 0$. Note that $\psi_m = 0 \implies \beta_m = 1 \implies m \geq 0 \implies S_n^-$ does not exist, and similarly $\psi_m = \pi \implies S_n^+$ does not exist. The formulae (79) and (80) (in which the terms in the sums are $O(|m|^{-n-1})$ for large $|m|$) are, to the best of our knowledge, new.

When $\beta = 0$, $\lambda_{2n-1} = -1/x$ and as $\beta \rightarrow 0$, $L_{2n} \rightarrow -1/x$. To see this write L_{2n} as a contour integral along the real line and then lift the contour above the pole at $u = i(\pi/2 - \arccos \beta)$. This shows that

$$L_{2n} = -\frac{(-1)^n \cos 2n\psi_0}{x \sin \psi_0} + \mathcal{A} \sin \beta x, \quad (84)$$

where \mathcal{A} is an integral which is bounded as $\beta \rightarrow 0$. It follows that in this case

$$S_{2n}^+ = S_{2n}^- = 2(-1)^n \sum_{m \geq 0} \frac{e^{2in\psi_m}}{x \sin \psi_m} + i\lambda_{2n} - \frac{1}{x} \quad (85)$$

$$= (-1)^n \sum_{m \in \mathbb{Z}} \frac{e^{2in \operatorname{sgn}(m)\psi_m}}{x \sin \psi_m} + i\lambda_{2n}, \quad (86)$$

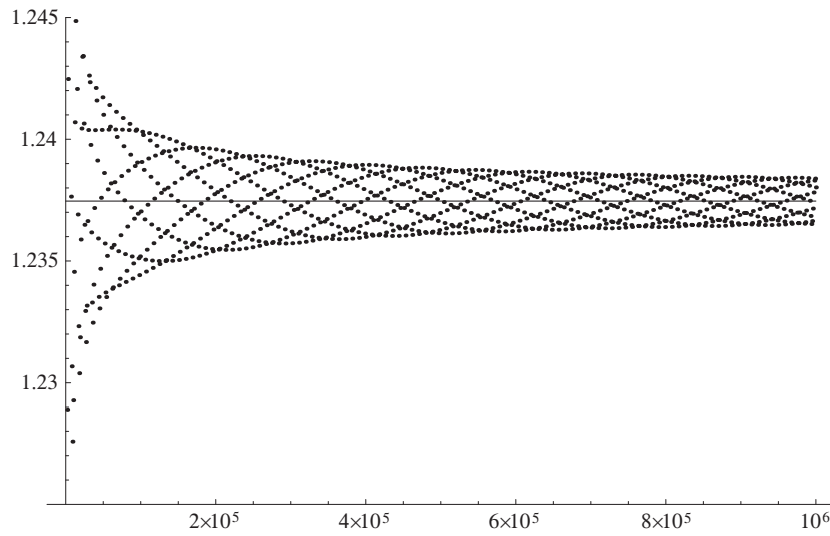


Figure 1. Computed values of $\text{Re } S_1^+(0.7, 0.5)$. The solid horizontal line represents the exact value (1.237 46 to six s.f.) computed via (79). The dots represent the partial sums computed from (1) in steps of 1000, up to 10^6 .

which agrees with (42), and

$$S_{2n-1}^+ = S_{2n-1}^- = 2i(-1)^n \sum_{m \geq 0} \frac{e^{i(2n-1)\psi_m}}{x \sin \psi_m} + iL_{2n-1} - \frac{1}{x} \tag{87}$$

$$= i(-1)^n \sum_{m \in \mathbb{Z}} \text{sgn}(m) \frac{e^{i(2n-1)\text{sgn}(m)\psi_m}}{x \sin \psi_m} + iL_{2n-1}, \tag{88}$$

which is new. When $\beta = \pi/x$, we also have $S_n^+ = S_n^-$ and this follows immediately from (79) and (80), since $\lambda_{2n-1} = 0$, $L_{2n} = 0$ (so $T_n^+ = T_n^-$) and from (14),

$$\sum_{m=-\infty}^{-1} \frac{e^{-in\psi_m}}{x \sin \psi_m} = \sum_{m=1}^{\infty} \frac{e^{-in(\pi-\psi_{m-1})}}{x \sin \psi_{m-1}} = (-1)^n \sum_{m=0}^{\infty} \frac{e^{in\psi_m}}{x \sin \psi_m}. \tag{89}$$

Two numerical examples will suffice. In figure 1, results are shown for $\text{Re } S_1^+$ when $x = 0.7$ and $\beta = 0.5$, while in figure 2 results are shown for $\text{Im } S_2^-$ when $x = 1.7$ and $\beta = 1.5$. The solid horizontal line in each case represents the exact value, computed via (79) and (80), these values being (to six significant figures (s.f.)) 1.237 46 and 0.639 241. The dots represent the partial sums computed from (1) in steps of 1000, up to 10^6 .

7. Connections with channel multipoles

In [13], solutions to the two-dimensional Helmholtz equation $\nabla^2\phi + k^2\phi = 0$ in a strip were constructed which are singular at the origin and which satisfy periodic boundary conditions on the edges of a strip. These functions are useful in solving scattering problems involving periodic arrays and they can be represented as a sum of images

$$\phi_n^s = \sum_{j \in \mathbb{Z}} H_n(kr_j) \cos n\theta_j e^{ij\chi^s} \tag{90}$$

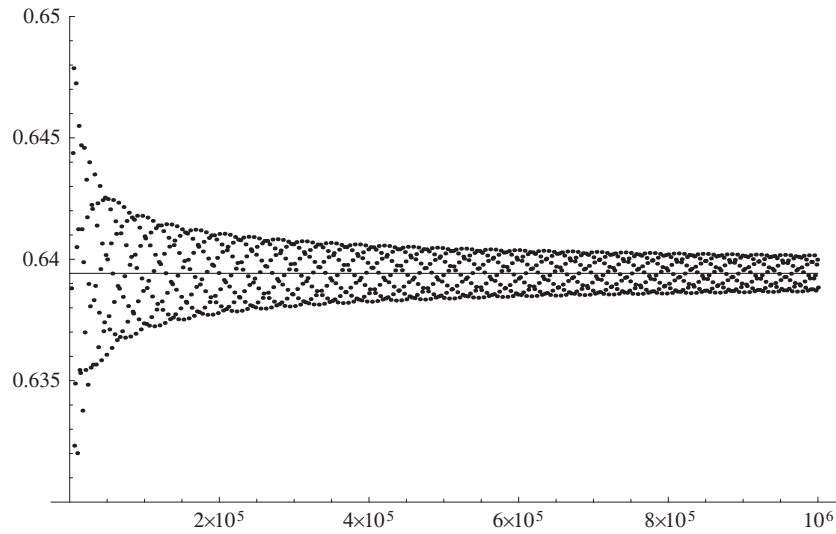


Figure 2. Computed values of $\text{Im } S_2^-(1.7, 1.5)$. The solid horizontal line represents the exact value (0.639 421 to six s.f.) computed via (80). The dots represent the partial sums computed from (1) in steps of 1000, up to 10^6 .

and

$$\phi_n^a = \sum_{j \in \mathbb{Z}} H_n(kr_j) \sin n\theta_j e^{ij\chi s}, \quad (91)$$

where s is the width of the strip, χ is an arbitrary phase factor, and (r_j, θ_j) are polar coordinates centred at $X = js, Y = 0$. (Note that here the angles θ_j are measured from the line of images, whereas in [13] they were measured from the normal to that line. In order to compare directly with that paper we would need to replace θ_j by $\pi/2 - \theta_j$.)

In order to use these functions near the origin, we expand them in terms of (r, θ) :

$$\phi_n^s = H_n(kr) \cos n\theta + \sum_{m=0}^{\infty} E_{m,n}^s J_m(kr) \cos m\theta \quad (92)$$

and

$$\phi_n^a = H_n(kr) \sin n\theta + \sum_{m=1}^{\infty} E_{m,n}^a J_m(kr) \sin m\theta, \quad (93)$$

and in [13] integral representations were derived for (the equivalent of) the coefficients $E_{m,n}$. The case $\chi = 0$ was treated in [14].

We can derive expressions for $E_{m,n}$ in terms of Schlömlich series as follows. Graf's addition theorem for Bessel functions [9, 8.530] allows us to write, for $r < |j|s$,

$$H_n(kr_j) \cos n\theta_j = \frac{1}{2} \sum_{m \in \mathbb{Z}} Q_{nm}^j (H_{n-m}(k|j|s) + (-1)^m H_{n+m}(k|j|s)) J_m(kr) e^{im\theta}, \quad (94)$$

where

$$Q_{nm}^j = \begin{cases} (-1)^{n+m} & j > 0 \\ 1 & j < 0 \end{cases} \quad (95)$$

and

$$H_n(kr_j) \sin n\theta_j = \frac{1}{2i} \sum_{m \in \mathbb{Z}} Q_{nm}^j (H_{n-m}(k|j|s) - (-1)^m H_{n+m}(k|j|s)) J_m(kr) e^{im\theta}. \quad (96)$$

It then follows that if we make the associations $\beta = \chi/k$ and $x = ks$,

$$\phi_n^s = H_n(kr) \cos n\theta + \sum_{m=0}^{\infty} \frac{\epsilon_m}{2} (\sigma_{n+m} + (-1)^m \sigma_{n-m}) J_m(kr) \cos m\theta, \quad (97)$$

where $\epsilon_0 = 1$ and $\epsilon_m = 2$ for $m > 0$, and

$$\phi_n^a = H_n(kr) \sin n\theta + \sum_{m=1}^{\infty} (\sigma_{n+m} - (-1)^m \sigma_{n-m}) J_m(kr) \sin m\theta. \quad (98)$$

Hence the coefficients $E_{m,n}$ can be computed using the expressions given in section 3. The integral representations derived in section 5 can be used with (97) and (98) to derive integral representations for $E_{m,n}$ which are equivalent to those given in [14] and [13].

8. Conclusion

The Schlömilch series defined in (1) are fundamental objects in the study of the diffraction of waves by semi-infinite periodic structures, but in order to compute them quickly and accurately alternative representations are required. In this paper we have collected together the known results and, via the use of integral representations and other methods, derived new ones. Equations (79) and (80) offer an efficient means of computing S_n^\pm for $n > 0$ and for $n = 0$ we can use (36) and (37). For $n = 0$, we have a convergence rate of $m^{-2} \ln |m|$ for the terms in the sum, whereas for $n > 0$ the terms decay like m^{-n-1} , though the series can be easily accelerated if necessary. For $n > 0$, we also need to evaluate an exponentially convergent integral.

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