PROCEEDINGS A

rspa.royalsocietypublishing.org

Research

CrossMark
click for updates

Cite this article: Asatryan AA. 2015 Summation of a Schlömilch type series. *Proc. R. Soc. A* **471**: 20150359.
http://dx.doi.org/10.1098/rspa.2015.0359

Received: 30 May 2015
Accepted: 22 October 2015

Subject Areas:
mathematical physics, optics, wave motion

Keywords:
conditionally converging series, multiple scattering, lattice sums

Author for correspondence:
A. A. Asatryan
e-mail: ara.asatrian@uts.edu.au

Electronic supplementary material is available at http://dx.doi.org/10.1098/rspa.2015.0359 or via http://rspa.royalsocietypublishing.org.

THE ROYAL SOCIETY PUBLISHING

Summation of a Schlömilch type series

A. A. Asatryan

School of Mathematical and Physical Sciences, University of Technology Sydney, Sydney New South Wales 2007, Australia

The ability to accurately and efficiently characterize multiple scattering of waves of different nature attracts substantial interest in physics. The advent of photonic crystals has created additional impetus in this direction. An efficient approach in the study of multiple scattering originates from the Rayleigh method, which often requires the summation of conditionally converging series. Here summation formulae have been derived for conditionally convergent Schlömilch type series $\sum_{s=-\infty}^{\infty} Z_n(|sD-x|) \times \mathrm{e}^{-\mathrm{i}n\arg(sD-x)}\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0}$, where $Z_n(z)$ stands for any of the following cylindrical functions of integer order: Bessel functions $J_n(z)$, Neumann functions $Y_n(z)$ or Hankel functions of the first kind $H_n^{(1)}(z) = J_n(z) + \mathrm{i}Y_n(z)$. These series arise in two-dimensional scattering problems on diffraction gratings with multiple inclusions per unit cell. It is shown that the Schlömilch series involving Hankel functions or Neumann functions can be expressed as an absolutely converging series of elementary functions and a finite sum of Lerch transcendent functions, while the Schlömilch series of Bessel functions can be transformed into a finite sum of elementary functions. The closed-form expressions for the Coates's integrals of integer order have also been found. The derived equations have been verified numerically and their accuracy and efficiency has been demonstrated.

1. Introduction

The primary purpose of this paper is to present summation formulae for conditionally convergent Schlömilch type series

$$S_n^Z(x) = \sum_{s=-\infty}^{\infty} Z_n(|sD-x|)\,\mathrm{e}^{-\mathrm{i}n\arg(sD-x)}\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0}, \qquad (1.1)$$

where $Z_n(z)$ stands for the following cylindrical functions of integer order n: Bessel functions $J_n(z)$, Neumann functions $Y_n(z)$ or Hankel functions of the first kind $H_n^{(1)}(z) = J_n(z) + \mathrm{i}Y_n(z)$ [1]. Here x and D are real numbers such that $0 < |x| < D$ and $0 \le \sin\theta_0 < 1$. The series (1.1) is an extremely slow, conditionally convergent series. Its partial sums are highly oscillatory (see §6) and the direct summation of the series (1.1) is meaningless. The series (1.1) converges provided $D(1 - \sin\theta_0)/2\pi$ and $D(1 + \sin\theta_0)/2\pi$ are not integers. The summation equation for the particular series (1.1) involving Bessel functions $J_n(z)$ of an even order n is given in [2]. Summation equations for general types of series (1.1) have not been derived until now.

Meanwhile, the summation of series (1.1) has both considerable theoretical interest and important applications in physics. For example, the series (1.1) arises naturally in two-dimensional scattering problems of plane waves on diffraction gratings composed of multiple inclusions per unit cell [3–5]. In this context, θ_0 is the angle of a plane wave incident on a grating measured from the normal to the grating. The parameter D is given by $D = kd = 2\pi d/\lambda$, while $x = kc_{lq}$, where $|c_{lq}|$ represents the distance between two inclusions in a grating unit cell. Here d is the grating period and λ is the radiation wavelength. In physical applications, the Schlömilch series are often called the lattice sums and they characterize the contribution to the wave's scattering amplitude at the vicinity of an inclusion l from an inclusion q and all its periodic replicas.

Recently, we have witnessed the emergence of the field of photonic [6,7] and phononic [8] crystals. Such structures can be viewed as a stack of diffraction gratings. Therefore, the ability to effectively and accurately characterize grating structures has become even more important in the broader context of applications in photonic and phononic crystals. A typical approach of modelling such structures requires the consideration of a unit cell with multiple inclusions [9,10]. By introducing intricate defects into such consecutive gratings, it is possible to model wave transport through rather complicated interconnected nano-scale networks of waveguides and resonators embedded in such crystals.

An analogous series to (1.1) with $x = 0$ appears in plane wave scattering problems on diffraction gratings with a single inclusion per unit cell

$$\tilde{S}_n = \sum_{s'=-\infty}^{\infty} H_n^{(1)}(|s|D)\,\mathrm{e}^{-\mathrm{i}n\arg(sD)}\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0}, \tag{1.2}$$

where the tilde over the summation variable s means that the term with $s = 0$ is absent from the series. The summation equation of series (1.2) at normal incidence $\theta_0 = 0$ was first given by von Ignatovsky [11,12]. By using intricate algebraic transformations von Ignatovsky expressed the series in terms of an absolutely converging series of elementary functions and a finite sum consisting of Bernoulli numbers B_m. Von Ignatovsky's result has been generalized for off-axis incidence $\theta_0 \neq 0$ in an elegant approach developed by Twersky [13]. It is shown there that, for the off-axis case, the series (1.2) can be expressed as a finite sum of Bernoulli polynomials $B_m(x)$ and an absolutely converging series of elementary functions. Twersky used Euler's summation formula in the form given by Nörlund [14] to deduce his final results [13]. Summation formulae of the zero order series ($n = 0$) (1.2) were included in major reference books for a while [2,15]; the summation formulae for more general series (1.2) are yet to be included.

In [3], Graf's addition theorem [16] has been used to convert the initial series (1.1) into the form

$$S_n^H(x) = \begin{cases} H_n^{(1)}(|x|) + \displaystyle\sum_{m=-\infty}^{\infty} (-1)^m \tilde{S}_{n+m} J_m(|x|) & \text{if } x < 0, \\[2ex] (-1)^n H_n^{(1)}(|x|) + \displaystyle\sum_{m=-\infty}^{\infty} \tilde{S}_{n+m} J_m(|x|) & \text{if } x > 0, \end{cases} \tag{1.3}$$

which allows numerical evaluation. For the numerical calculation to converge, series (1.3) can be truncated at values $m \lesssim |x|$ for $n \lesssim 10$. In typical cases, approximately $-100 \le m \le 100$ terms are required to achieve convergence in (1.3). Therefore, use of (1.3) requires calculation of $\tilde{S}_n$ of up to order $n \approx 100$. While equation (1.3) is quite efficient for the summation of the series (1.1) for $D \lesssim 100$, this method loses accuracy for larger values of D. The deficiency associated with equation (1.3) is that the sum in (1.3) contained the product of increasing $\tilde{S}_m$ and decreasing $J_m(|x|)$ factors, which leads to the loss of accuracy for larger D.

The ability to model structures with larger unit cells which can accommodate more inclusions has broad and important applications. These applications include, for example, the characterization of wave transport through complex waveguide structures embedded in photonic crystals, consideration of the effects of manufacturing imperfections on operational properties of devices embedded in such crystals or the study of the fundamental problem of Anderson localization of waves in disordered media [17–19]. As it was once well stated—*more is different* [20].

Therefore, it is important and interesting both analytically and from an application perspective to derive Ignatovsky–Twersky like formulae that can be used to directly find values of $S_n^Z(x)$ accurately and efficiently for substantially larger values of $D \gg 100$. In this paper, we adopt the approach developed by Twersky [13] and derive such summation formulae for the series (1.1). It is shown here that the Schlömilch series (1.1) involving Hankel functions or Neumann functions can be expressed as a finite sum of Lerch transcendent functions $\Phi(z,s,v)$ and an absolutely converging elementary series. For the particular case of normal incidence $\theta_0 = 0$, the Schlömilch series (1.1) of Hankel functions or Neumann functions can be expressed as a finite sum involving polylogarithm functions $Li_s(z)$ and an absolutely converging elementary series. The summation formulae for the Schlömilch series (1.1) involving Bessel functions have also been derived and are expressed in terms of a finite sum of elementary functions only. For the reported result in [2] for the even order series, $S_{2n}^J(x)$ has been reproduced. Closed-form expressions for Coates's integrals [21] of integer order, which are also required for the derivation of the summation formulae, have been found in the process.

First, in §2 the key relations are derived, which are used subsequently in §3 to find the summation formulae for the series $S_n^H(x)$. The derivation of the summation formulae for $S_n^J(x)$ and $S_n^Y(x)$ series are presented in §4, while the normal incidence case is considered in §5. The numerical verification, accuracy and efficiency of the derived summation formulae have been considered in §6. Derivation of the closed-form expressions of the required integrals over a finite interval are given in appendix A, while the electronic supplementary material describes the derivation of the closed-form expressions for Coates's integrals of integer order.

2. Derivation of the basic relations

In this section, the basic relations are derived, which are used subsequently to transform series (1.1) into a form which allows efficient and accurate summation of the series $S_n^Z(x)$. First, it is easy to see the relation between negative and positive orders of the series $S_n^Z(x)$

$$S_{-n}^Z(x) = (-1)^n S_n^Z(x), \tag{2.1}$$

which can be proved by replacing $n \to -n$ in (1.1) and observing that $\arg(-x + sD)$ is either zero or π. Therefore, it is sufficient to derive the summation formulae for only non-negative orders $n \geq 0$ and the negative orders $n < 0$ can be deduced using equation (2.1). Relation (2.1) also holds for the series (1.2) for the same reason.

By direct inspection of series (1.1), it can be established that $S_n^Z(x)$ is quasi-periodic and satisfies the relation

$$S_n^Z(x + D) = S_n^Z(x)\,\mathrm{e}^{\mathrm{i}D\sin\theta_0}. \tag{2.2}$$

By replacing x with $-x$ in (2.2), it is easy to establish the relation

$$S_n^Z(-x) = S_n^Z(D - x)\,\mathrm{e}^{-\mathrm{i}D\sin\theta_0}, \tag{2.3}$$

which provides a connection between the values for $S_n^Z(x)$ for positive and negative arguments. Therefore, it is sufficient to derive summation formulae for $S_n^Z(x)$ with only positive values of argument x, while the values for $S_n^Z(x)$ with negative arguments can be calculated using relation (2.3). Nevertheless, in subsequent derivations we will not require x to be positive.

First, we consider the series $S_n^H(x)$ involving Hankel functions. The beginning of the derivation is similar to Twersky's approach [13], but for the reader's convenience and for an introduction to the nomenclature, we provide it here. Following [13], we consider the series

$$h_n(x,y) = \sum_{s=-\infty}^{\infty} H_n^{(1)}(R_s)\,\mathrm{e}^{-\mathrm{i}n\varphi_s}\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0}, \tag{2.4}$$

where

$$\mathbf{R}_s = (sD-x)\hat{e}_x + y\hat{e}_y, \quad \varphi_s = \arg(\mathbf{R}_s) \quad R_s = \sqrt{(sD-x)^2+y^2} \tag{2.5}$$

and $\hat{e}_x$, $\hat{e}_y$ are unit vectors along the x- and y-axes. Therefore,

$$S_n^H(x) = \lim_{y\to 0} h_n(x,y), \tag{2.6}$$

given $R_s \to |sD-x|$ as $y\to 0$. For $y>0$ and using Sommerfeld integral representation of the Hankel function, we can write

$$H_n^{(1)}(R_s)\,\mathrm{e}^{-\mathrm{i}n\arg(\mathbf{R}_s)} = \frac{(-1)^n}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}(sD-x)t+\mathrm{i}y\sqrt{1-t^2}+\mathrm{i}n\arcsin t}}{\sqrt{1-t^2}}\mathrm{d}t, \tag{2.7}$$

where $\sqrt{1-t^2} = \mathrm{i}\sqrt{t^2-1}$ for $|t|>1$. After substitution of (2.7) into (2.4) and using either the Poisson summation formula

$$\frac{1}{2\pi}\sum_{s=-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}sa}\int_{-\infty}^{\infty} f(t)\,\mathrm{e}^{\mathrm{i}st}\mathrm{d}t = \sum_{p=-\infty}^{\infty} f(a-2\pi p) \tag{2.8}$$

or the identity

$$\sum_{s=-\infty}^{\infty}\mathrm{e}^{\mathrm{i}sD(t+\sin\theta_0)} = 2\pi\sum_{p=-\infty}^{\infty}\delta(Dt+D\sin\theta_0-2\pi p), \tag{2.9}$$

we deduce the following relation

$$\sum_{s=-\infty}^{\infty} H_n^{(1)}(R_s)\,\mathrm{e}^{-\mathrm{i}n\arg(\mathbf{R}_s)}\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0} = 2\sum_{p=-\infty}^{\infty}\frac{(-1)^n\,\mathrm{e}^{-\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p+\mathrm{i}y\cos\theta_p}}{D\cos\theta_p} \tag{2.10}$$

applicable for $y>0$. Here the angles θ_p given by the relation

$$\sin\theta_p = \sin\theta_0 + \frac{2\pi p}{D}, \quad p = 0, \pm 1, \pm 2, \ldots \tag{2.11}$$

represent the diffraction orders of plane waves in grating terminology. The representation of (2.4) for $y<0$ is obtained from (2.10) by replacing θ_p by $\pi-\theta_p$ and it takes the form

$$\sum_{s=-\infty}^{\infty} H_n^{(1)}(R_s)\,\mathrm{e}^{-\mathrm{i}n\arg(\mathbf{R}_s)}\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0}=2\sum_{p=-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p-\mathrm{i}y\cos\theta_p}}{D\cos\theta_p},\quad y<0. \tag{2.12}$$

The series (2.10) and (2.12) converge if

$$\frac{D(1\mp\sin\theta_0)}{2\pi}=m_\pm\neq 0,1,2,\ldots. \tag{2.13}$$

There are two kinds of diffraction orders in (2.11), the propagating orders and evanescent orders. For propagating orders $|\sin\theta_p|<1$ and $-p_-\le p\le p_+$, where $p_\pm=[m_\pm]=[D(1\mp\sin\theta_0)/2\pi]$ are the largest integers smaller than $m_\pm$. The rest of the orders $p\ge p_++1>m_+$ and $p\le -p_--1<-m_-$ are evanescent orders satisfying $|\sin\theta_p|>1$. For $p\ge p_++1$ we have $\theta_p=\pi/2-\mathrm{i}|\eta_p|$ and for $p\le -p_--1$ we have $\theta_p=-\pi/2+\mathrm{i}|\eta_p|$, where $\cosh\eta_p=\sin\theta_0+2\pi p/D$. The values $\sin\theta_p=\pm 1$, where $m_\pm=0,1,2,\ldots$ correspond to the Rayleigh wavelength values in which the diffracted wave propagates along the surface of a grating.

For $n=0$, both of the relations (2.10) and (2.12) reduce to

$$\sum_{s=-\infty}^{\infty} H_0^{(1)}(R_s)\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0}=2\sum_{p=-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}x\sin\theta_p+\mathrm{i}|y|\cos\theta_p}}{D\cos\theta_p}, \tag{2.14}$$

which is the spectral representation of the periodic Green's function considered previously in a number of references (e.g. [22–25]). The spectral decomposition (2.14) is applicable for $y=0$, which coincides with the initial series (1.1) for zero order $S_0^H(x)$ given by

$$S_0^H(x)=\sum_{s=-\infty}^{\infty} H_0^{(1)}(|sD-x|)\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0} \tag{2.15}$$

$$=2\sum_{p=-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}x\sin\theta_p}}{D\cos\theta_p}. \tag{2.16}$$

Although the spectral form of the series (2.16) converges marginally better than the original series (2.15), the convergence of series (2.16) can be substantially accelerated using one of the forms of the Kummer transformation [26,27]. For a review on this subject, see [28]. In the subsequent calculations, we assume that the order of the series n is positive, $n>0$ unless stated otherwise.

3. Summation formula for $S_n^H(x)$

In this section, we derive the summation formulae for the series $S_n^H(x)$. First, we derive the key relation based on the integral representation of the Hankel functions (2.7) and the sum of the Hankel functions (2.10) and (2.12).

(a) The derivation of the key relation

We use the integral representation of Hankel's function

$$H_n^{(1)}(R_0)\,\mathrm{e}^{-\mathrm{i}n\varphi_0}=2\int_{-\infty}^{\infty}\frac{(-1)^n\,\mathrm{e}^{-\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p+\mathrm{i}y\cos\theta_p}}{D\cos\theta_p}\mathrm{d}p,\quad y>0 \tag{3.1}$$

and

$$H_n^{(1)}(R_0)\,\mathrm{e}^{-\mathrm{i}n\varphi_0}=2\int_{-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p-\mathrm{i}y\cos\theta_p}}{D\cos\theta_p}\mathrm{d}p,\quad y<0 \tag{3.2}$$

to regularize the series in (2.10) and (2.12), respectively, as we take the limit $y \to 0$. First, we add and subtract the Hankel function from the series (2.10) and (2.12) to deduce

$$h_n(x,y) = 2\left(\sum_{p=-\infty}^{\infty} - \int_{-\infty}^{\infty} \mathrm{d}p\right) \frac{(-1)^n\,\mathrm{e}^{-\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p + \mathrm{i}y\cos\theta_p}}{D\cos\theta_p} + H_n^{(1)}(R_0)\,\mathrm{e}^{-\mathrm{i}n\arg(\mathbf{R}_0)}, \quad y > 0 \tag{3.3}$$

and

$$h_n(x,y) = 2\left(\sum_{p=-\infty}^{\infty} - \int_{-\infty}^{\infty} \mathrm{d}p\right) \frac{\mathrm{e}^{\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p - \mathrm{i}y\cos\theta_p}}{D\cos\theta_p} + H_n^{(1)}(R_0)\,\mathrm{e}^{-\mathrm{i}n\arg(\mathbf{R}_0)}, \quad y < 0. \tag{3.4}$$

Now we substitute (3.4) into (2.6) and denote $\pm y = \varepsilon \to 0$ and obtain

$$\begin{aligned} S_n^H(x) &= \lim_{\varepsilon\to 0} 2\left(\sum_{p=-\infty}^{\infty} - \int_{-\infty}^{\infty} \mathrm{d}p\right) \mathrm{e}^{\mathrm{i}\varepsilon\cos\theta_p} \frac{\mathrm{e}^{\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + H_n^{(1)}(|x|)\,\mathrm{e}^{-\mathrm{i}n\arg(-\mathbf{x})} \\ &\equiv 2\mathsf{S}\frac{\mathrm{e}^{\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + H_n^{(1)}(|x|)\,\mathrm{e}^{-\mathrm{i}n\arg(-\mathbf{x})}, \end{aligned} \tag{3.5}$$

where we have introduced the Nörlund operator S [14].

Next, we split the first term in (3.5) into two terms

$$\begin{aligned} S_n^H(x) &= 2\mathsf{S}\frac{\mathrm{e}^{\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + H_n^{(1)}(|x|)\,\mathrm{e}^{-\mathrm{i}n\arg(-\mathbf{x})} \\ &= 2\mathsf{S}_-\frac{\mathrm{e}^{\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + 2\mathsf{S}_+\frac{\mathrm{e}^{\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + H_n^{(1)}(|x|)\,\mathrm{e}^{-\mathrm{i}n\arg(-\mathbf{x})}, \end{aligned} \tag{3.6}$$

where

$$\mathsf{S}_- f(p) = \lim_{\varepsilon\to 0}\left(\sum_{p=-\infty}^{-1} - \int_{-\infty}^{-\Delta\sin\theta_0} \mathrm{d}p\right) f(p)\,\mathrm{e}^{\mathrm{i}\varepsilon\cos\theta_p}, \tag{3.7}$$

$$\mathsf{S}_+ f(p) = \lim_{\varepsilon\to 0}\left(\sum_{p=0}^{\infty} - \int_{-\Delta\sin\theta_0}^{\infty} \mathrm{d}p\right) f(p)\,\mathrm{e}^{\mathrm{i}\varepsilon\cos\theta_p} \tag{3.8}$$

and $\Delta = D/2\pi$. Then we add and subtract the term $(-1)^n\,\mathrm{e}^{-\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p}$ in the kernel of S_+ and introduce the $F_n(x)$ term

$$F_n(x) = 2\mathsf{S}_+\frac{[\mathrm{e}^{\mathrm{i}n\theta_p} - (-1)^n\,\mathrm{e}^{-\mathrm{i}n\theta_p}]\,\mathrm{e}^{\mathrm{i}x\sin\theta_p}}{D\cos\theta_p}. \tag{3.9}$$

Equation (3.6) takes the form

$$S_n^H(x) = 2\mathsf{S}_-\frac{\mathrm{e}^{\mathrm{i}n\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + 2\mathsf{S}_+\frac{\mathrm{e}^{\mathrm{i}n(\pi-\theta_p) + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + F_n(x) + H_n^{(1)}(|x|)\,\mathrm{e}^{-\mathrm{i}n\arg(-\mathbf{x})}. \tag{3.10}$$

The convergence factor $\mathrm{e}^{\mathrm{i}\varepsilon\cos\theta_p}$ is not required for the two first terms in (3.10). Therefore, we take $\varepsilon = 0$ in these terms and split the integrals over the propagating orders and evanescent orders and, after changing the variable of integration to θ_p, we deduce

$$
\begin{aligned}
S_n^H(x) = {} & 2\sum_{p=-\infty}^{-1} \frac{\mathrm{e}^{\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + 2\sum_{p=0}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\pi n-\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p}}{D\cos\theta_p} - \frac{1}{\pi}\int_0^{\pi/2} \mathrm{e}^{-\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p}\,\mathrm{d}\theta_p \\
& - \frac{(-1)^n}{\pi}\int_0^{\pi/2} \mathrm{e}^{-\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p}\,\mathrm{d}\theta_p - \frac{1}{\pi}\int_{-\pi/2+\mathrm{i}\infty}^{-\pi/2} \mathrm{e}^{\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p}\,\mathrm{d}\theta_p \\
& - \frac{(-1)^n}{\pi}\int_{\pi/2}^{\pi/2-\mathrm{i}\infty} \mathrm{e}^{-\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p}\,\mathrm{d}\theta_p + F_n(x) + H_n^{(1)}(|x|)\,\mathrm{e}^{-\mathrm{i}n\arg(-\mathbf{x})}.
\end{aligned} \tag{3.11}
$$

The integration parallel to the imaginary axis in the last two integrals in (3.11) can be converted to integrals over a real variable using the parametrization $\theta_p = \mp\pi/2 \pm it$. This leads to the following representation of (3.11)

$$
\begin{aligned}
S_n^H(x) = {} & 2\sum_{p=-\infty}^{-1} \frac{\mathrm{e}^{\mathrm{i}n\theta_p-\mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + 2\sum_{p=0}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\pi n-\mathrm{i}n\theta_p-\mathrm{i}x\sin\theta_p}}{D\cos\theta_p} - \frac{1}{\pi}\int_0^{\pi/2} \mathrm{e}^{-\mathrm{i}n\theta_p-\mathrm{i}x\sin\theta_p}\,\mathrm{d}\theta_p \\
& - \frac{(-1)^n}{\pi}\int_0^{\pi/2} \mathrm{e}^{-\mathrm{i}n\theta_p+\mathrm{i}x\sin\theta_p}\,\mathrm{d}\theta_p + \frac{\mathrm{i}}{\pi}\,\mathrm{e}^{-\mathrm{i}\pi n/2}\int_0^{\infty} \mathrm{e}^{-nt-\mathrm{i}x\cosh t}\,\mathrm{d}t \\
& + \frac{\mathrm{i}(-1)^n}{\pi}\,\mathrm{e}^{-\mathrm{i}\pi n/2}\int_0^{\infty} \mathrm{e}^{-nt+\mathrm{i}x\cosh t}\,\mathrm{d}t + F_n(x) + H_n^{(1)}(|x|)\,\mathrm{e}^{-\mathrm{i}n\arg(-\mathbf{x})}.
\end{aligned} \tag{3.12}
$$

The subsequent calculations are more convenient to carry out for even and odd order values of n separately.

For even n, we combine the last two integrals over the infinite region together and the first two integrals over a finite region together in (3.12) then expand the factor $\mathrm{e}^{-\mathrm{i}n\theta_p}$ into its trigonometric parts, which leads to

$$
\begin{aligned}
S_{2n}^H(x) = {} & 2\sum_{p=-\infty}^{-1} \frac{\mathrm{e}^{\mathrm{i}2n\theta_p+\mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + 2\sum_{p=0}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}2n\theta_p+\mathrm{i}x\sin\theta_p}}{D\cos\theta_p} - \frac{2}{\pi}\int_0^{\pi/2} \cos(x\sin\theta_p)\cos(2n\theta_p)\,\mathrm{d}\theta_p \\
& + \frac{2\mathrm{i}}{\pi}\int_0^{\pi/2} \cos(x\sin\theta_p)\sin(2n\theta_p)\,\mathrm{d}\theta_p + \frac{2\mathrm{i}(-1)^n}{\pi}\int_0^{\infty} \cos(x\cosh t)\,\mathrm{e}^{-2nt}\,\mathrm{d}t + F_{2n}(x) \\
& + H_{2n}^{(1)}(|x|)\,\mathrm{e}^{-\mathrm{i}2n\arg(-\mathbf{x})}.
\end{aligned} \tag{3.13}
$$

The phase factor $\mathrm{e}^{-\mathrm{i}2n\arg(\mathbf{x})}$ of the Hankel function $H^{(1)}(|x|)$ in (3.13) can be dropped, given it is equal to unity regardless of the sign of x. Now using the Bessel function representation ([2], p. 79)

$$
J_{2n}(|x|) = \frac{2}{\pi}\int_0^{\pi/2} \cos(x\sin\theta_p)\cos(2n\theta_p)\,\mathrm{d}\theta_p, \tag{3.14}
$$

the Bessel part $J_{2n}(x)$ of the Hankel $H_{2n}^{(1)}(|x|)$ function in (3.13) is cancelled and we deduce

$$
\begin{aligned}
S_{2n}^H(x) = {} & 2\sum_{p=-\infty}^{-1} \frac{\mathrm{e}^{\mathrm{i}2n\theta_p+\mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + 2\sum_{p=0}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}2n\theta_p+\mathrm{i}x\sin\theta_p}}{D\cos\theta_p} + \frac{2\mathrm{i}}{\pi}\int_0^{\pi/2} \cos(x\sin\theta_p)\sin(2n\theta_p)\,\mathrm{d}\theta_p \\
& + \frac{2\mathrm{i}(-1)^n}{\pi}\int_0^{\infty} \cos(x\cosh t)\,\mathrm{e}^{-2nt}\,\mathrm{d}t + F_{2n}(x) + \mathrm{i}Y_{2n}(|x|).
\end{aligned} \tag{3.15}
$$

For odd vales of n, we combine the integrals over the infinite region together in (3.12) and we combine the first two integrals over the finite region together. Then we expand the factor $\mathrm{e}^{-\mathrm{i}(2n+1)\theta_p}$ into its trigonometric parts transforming (3.12) into

$$\begin{aligned} S^H_{2n+1}(x) = {} & 2\sum_{p=-\infty}^{-1} \frac{\mathrm{e}^{\mathrm{i}(2n+1)\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} - 2\sum_{p=0}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(2n+1)\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} \\ & + \frac{2}{\pi}\int_0^{\pi/2} \sin(x\sin\theta_p)\sin(2n+1)\theta_p \,\mathrm{d}\theta_p + \frac{2\mathrm{i}}{\pi}\int_0^{\pi/2} \sin(x\sin\theta_p)\cos(2n+1)\theta_p\,\mathrm{d}\theta_p \\ & + \frac{2\mathrm{i}(-1)^n}{\pi}\int_0^{\infty} \sin(x\cosh t)\,\mathrm{e}^{-(2n+1)t}\,\mathrm{d}t + F_{2n+1}(x) + H^{(1)}_{2n+1}(|x|)\,\mathrm{e}^{-\mathrm{i}(2n+1)\arg(-\mathbf{x})}. \end{aligned} \tag{3.16}$$

Now we note that the first integral in (3.16) can be expressed in terms of the Bessel function $J_{2n+1}(x)$ ([2], p. 79)

$$J_{2n+1}(|x|)\,\mathrm{e}^{\mathrm{i}(2n+1)\arg(x)} = \frac{2}{\pi}\int_0^{\pi/2} \sin(x\sin\theta_p)\sin(2n+1)\theta_p\,\mathrm{d}\theta_p. \tag{3.17}$$

Therefore, (3.16) takes the form

$$\begin{aligned} S^H_{2n+1}(x) = {} & 2\sum_{p=-\infty}^{-1} \frac{\mathrm{e}^{\mathrm{i}(2n+1)\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} - 2\sum_{p=0}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(2n+1)\theta_p + \mathrm{i}x\sin\theta_p}}{D\cos\theta_p} \\ & + \frac{2\mathrm{i}}{\pi}\int_0^{\pi/2} \sin(x\sin\theta_p)\cos(2n+1)\theta_p\,\mathrm{d}\theta_p - \frac{2\mathrm{i}(-1)^n}{\pi}\int_0^{\infty} \sin(x\cosh t)\,\mathrm{e}^{-(2n+1)t}\,\mathrm{d}t \\ & + F_{2n+1}(x) + \mathrm{i}Y^{(1)}_{2n+1}(|x|)\,\mathrm{e}^{-\mathrm{i}(2n+1)\arg(-\mathbf{x})}, \end{aligned} \tag{3.18}$$

as the Bessel part $J_{2n+1}(|x|)$ of the Hankel function cancels given that integral (3.17) always has the opposite sign to the last term in (3.16).

It appears that the integrals over the infinite intervals in (3.15) and (3.18) were first considered by Coates in [21] and these integrals are also subsequently mentioned by Watson for more general cases of non-integer order n ([1], p. 313). It turns out that the Coates integrals appearing in equations (3.15) and (3.18) and integrals over the finite region in (3.15) and (3.18) can be calculated in closed form. The details of this calculation are given in appendix A and in the electronic supplementary material. In the next section, we provide details for the calculation of the $F_n(x)$ term using the limiting process based on the Nörlund summation formula [14].

(b) Calculation of the $F_n(x)$ term

The first two series in (3.10) converge without requiring the application of a convergence limiting process. By contrast, the $F_n(x)$ term is calculated by using the Nörlund summation formula [14] expressed in the form

$$\lim_{\varepsilon\to 0}\left\{\int_0^{\infty} z^{n-1}\,\mathrm{e}^{-\varepsilon z}\,\mathrm{d}z - \sum_{s=0}^{\infty}(s+x)^{n-1}\,\mathrm{e}^{-(s+x)\varepsilon}\right\} = \frac{B_n(x)}{n}, \tag{3.19}$$

where $B_n(x)$ is a Bernoulli polynomial. In the subsequent calculations, we use the following form of relation (3.19)

$$\begin{aligned} \mathsf{S}_{+}(p+\Delta\sin\theta_0)^{n-1} &= \lim_{\varepsilon\to 0}\left(\sum_{p=0}^{\infty} - \int_{-\Delta\sin\theta_0}^{\infty}\mathrm{d}p\right)(p+\Delta\sin\theta_0)^{n-1}\,\mathrm{e}^{\mathrm{i}\varepsilon\cos\theta_p} \\ &= \frac{-B_n(\Delta\sin\theta_0)}{n}. \end{aligned} \tag{3.20}$$

Note that the convergence factor $\mathrm{e}^{\mathrm{i}\varepsilon\cos\theta_p}$ in (3.20) is equivalent to the convergence factor $\mathrm{e}^{-\varepsilon z}$ in (3.19), given $\cos\theta_p \sim \mathrm{i}p/\Delta$ for large values of p. We consider even and odd n cases separately. First, we derive the expression for $F_{2n}(x)$.

(i) Derivation of the expression for $F_{2n}(x)$

For even values of order n, $F_{2n}(x)$ takes the form

$$F_{2n}(x) = \frac{4\mathrm{i}}{D} \mathfrak{S}_+ \frac{\sin(2n\theta_p)}{\cos\theta_p}\,\mathrm{e}^{\mathrm{i}x\sin\theta_p}. \tag{3.21}$$

Now we expand the exponential factor $\mathrm{e}^{\mathrm{i}x\sin\theta_p}$ in (3.21) into a Taylor series and use the relation

$$\frac{\sin(2n\theta_p)}{\cos\theta_p} = \sum_{m=1}^{n} \frac{(-1)^{m-1}2^{2m-1}(n+m-1)!}{(2m-1)!(n-m)!} \sin^{2m-1}\theta_p \equiv \sum_{m=1}^{n} [n,m] \sin^{2m-1}\theta_p \tag{3.22}$$

to convert (3.21) into the form

$$F_{2n}(x) = \frac{4\mathrm{i}}{D} \sum_{m=1}^{n} \frac{[n,m]}{\Delta^{2m-1}} \sum_{q=0}^{\infty} \frac{(\mathrm{i}x/\Delta)^q}{q!} \mathfrak{S}_+ (p+\Delta\sin\theta_0)^{q+2m-1}. \tag{3.23}$$

After application of the Nörlund summation formula (3.20), expression (3.23) takes the form

$$F_{2n}(x) = -\frac{4\mathrm{i}}{D} \sum_{m=1}^{n} \frac{[n,m]}{\Delta^{2m-1}} \sum_{q=0}^{\infty} \frac{(\mathrm{i}x/\Delta)^q}{q!} \frac{B_{q+2m}(\Delta\sin\theta_0)}{q+2m}. \tag{3.24}$$

The series in (3.24) can be expressed in terms of the Lerch transcendent function $\Phi(z,s,\alpha)$ defined by [2,29]

$$\Phi(z,s,\alpha) = \sum_{n=0}^{\infty} \frac{z^n}{(n+\alpha)^s}. \tag{3.25}$$

Using the identity [29,30]

$$\sum_{k=0}^{\infty} \frac{t^k}{k!(k+n)} B_{k+n}(x) = (n-1)!(-t)^{-n} - \mathrm{e}^{tx}\Phi(\mathrm{e}^t, 1-n, x), \quad n=2,3,\ldots, \tag{3.26}$$

which is applicable for $|t| < 2\pi$, equation (3.24) can be written as

$$F_{2n}(x) = -\frac{2i}{\pi} \sum_{m=1}^{n} \frac{[n,m]}{\Delta^{2m}} \left[(2m-1)! \left(\frac{-\mathrm{i}x}{\Delta}\right)^{-2m} - \mathrm{e}^{\mathrm{i}x\sin\theta_0}\Phi(\mathrm{e}^{\mathrm{i}x/\Delta}, 1-2m, \Delta\sin\theta_0) \right]. \tag{3.27}$$

Note that the applicability condition of (3.26) is satisfied provided $|x|/D < 1$. The final expression for $F_{2n}(x)$ can be deduced from (3.27) after straightforward algebraic transformations

$$F_{2n}(x) = \frac{\mathrm{i}\,\mathrm{e}^{\mathrm{i}x\sin\theta_0}}{\pi} \sum_{m=1}^{n} \frac{(-1)^{m-1}2^{2m}(n+m-1)!}{\Delta^{2m}(2m-1)!(n-m)!} \Phi(\mathrm{e}^{\mathrm{i}x/\Delta}, 1-2m, \Delta\sin\theta_0)$$
$$+ \frac{\mathrm{i}}{\pi} \sum_{m=1}^{n} \frac{2^{2m}(n+m-1)!}{(n-m)!x^{2m}}. \tag{3.28}$$

Although x cannot take zero value in the initial sum $S_n^H(x)$, the term $F_{2n}(x)$ can be calculated for $x=0$. Using the limit [2]

$$\lim_{z\to 1} [\Phi(z,s,\alpha) - \Gamma(1-s)[-\log z]^{s-1} z^{-\alpha}] = \zeta(s,\alpha), \tag{3.29}$$

where

$$\zeta(s,\alpha) = \sum_{n=0}^{\infty} \frac{1}{(\alpha+n)^s} \tag{3.30}$$

is the generalized zeta or Hurwitz zeta function, the expression in the square bracket in (3.27) can be rewritten in terms of the Bernoulli polynomials using their connection with the generalized zeta function [29]

$$\zeta(1-2m, \Delta\sin\theta_0) = -\frac{B_{2m}(\Delta\sin\theta_0)}{2m}. \tag{3.31}$$

The substitution of (3.31) into (3.27) reproduces the corresponding term in Twersky's result [13]. This demonstrates the consistency of the obtained relation (3.28) with Twersky's result.

(ii) Derivation of the expression for $F_{2n+1}(x)$

The calculation for the odd order terms, $F_{2n+1}(x)$, is quite similar to the even order case. For odd values of n relation (3.9) takes the form

$$F_{2n+1}(x) = \frac{4}{D} \mathsf{S}_{+} \frac{\cos(2n+1)\theta_p}{\cos\theta_p} \mathrm{e}^{\mathrm{i}x\sin\theta_p}. \tag{3.32}$$

Now we use the identity

$$\frac{\cos(2n+1)\theta_p}{\cos\theta_p} = \sum_{m=0}^{n} \frac{(-1)^m 2^{2m}(n+m)!}{(2m)!(n-m)!} \sin^{2m}\theta_p \equiv \sum_{m=0}^{n} \{n,m\} \sin^{2m}\theta_p \tag{3.33}$$

and expand the exponential function $\mathrm{e}^{\mathrm{i}x\sin\theta_p}$ in (3.32) into a Taylor series and transform (3.32) into

$$F_{2n+1}(x) = \frac{2}{\pi\Delta} \sum_{m=0}^{n} \frac{\{n,m\}}{\Delta^{2m}} \sum_{q=0}^{\infty} \frac{(\mathrm{i}x/\Delta)^q}{q!} \mathsf{S}_{+}(p+\Delta\sin\theta_0)^{q+2m}. \tag{3.34}$$

Next, we apply the Nörlund summation formula (3.20) and express (3.34) in the form

$$\begin{aligned} F_{2n+1}(x) = &-\frac{2}{\pi\Delta} \sum_{q=0}^{\infty} \frac{(\mathrm{i}x/\Delta)^q}{q!} \frac{B_{q+1}}{q+1} \\ &-\frac{2}{\pi} \sum_{m=1}^{n} \frac{(-1)^m 2^{2m}(n+m)!}{(2m)!(n-m)!\Delta^{2m+1}} \sum_{q=0}^{\infty} \frac{(\mathrm{i}x/\Delta)^q}{q!} \frac{B_{q+2m+1}(\Delta\sin\theta_0)}{q+2m+1}. \end{aligned} \tag{3.35}$$

The first term in (3.35) can be simplified using the identity ([29], p. 25)

$$\sum_{k=0}^{\infty} B_n(x) \frac{t^{n-1}}{n!} = \frac{\mathrm{e}^{xt}}{\mathrm{e}^t - 1}, \quad |t| < 2\pi, \tag{3.36}$$

while the infinite sum in (3.35) can be calculated in closed form by using relation (3.26) in a similar way to that for the even n case. The final expression for $F_{2n+1}(x)$ takes the form

$$\begin{aligned} F_{2n+1}(x) = &-\frac{2i}{\pi x} - \frac{2i}{\pi} \sum_{m=1}^{n} \frac{2^{2m}(n+m)!}{(n-m)!x^{2m+1}} + \frac{2}{\pi\Delta} \frac{\mathrm{e}^{\mathrm{i}x\sin\theta_0}}{1-\mathrm{e}^{\mathrm{i}x/\Delta}} \\ &+ \frac{2}{\pi} \sum_{m=1}^{n} \frac{(-1)^m 2^{2m}(n+m)!}{(2m)!(n-m)!\Delta^{2m+1}} \mathrm{e}^{\mathrm{i}x\sin\theta_0} \Phi(\mathrm{e}^{\mathrm{i}x/\Delta}, -2m, \Delta\sin\theta_0). \end{aligned} \tag{3.37}$$

Similar to the even n case, expression (3.37) reduces to the corresponding term of Twersky's result [13] for $x = 0$.

(iii) Final forms of the series $S_n^H(x)$

The final expression for the series $S_n^H(x)$ can be written down now. For even n, we substitute expression (3.28) for $F_{2n}(x)$ and the values for integrals (A 4) and (A 9) into (3.15). Some pleasing cancellations occur. The double sums of integral (A 4) cancel the double sums of the Coates integral (A 9), while the Neumann function of the Coates integral (A 9) $Y_{2n}(|x|)$ cancels the corresponding term in (3.15). The second term of $F_{2n}(x)$ (3.28) cancels the last term of integral (A 4) and the expression for $S_{2n}^H(x)$ takes the final form

$$S_{2n}^H(x) = 2\sum_{p=-\infty}^{-1} \frac{e^{i2n\theta_p + ix\sin\theta_p}}{D\cos\theta_p} + 2\sum_{p=0}^{\infty} \frac{e^{-i2n\theta_p + ix\sin\theta_p}}{D\cos\theta_p} + \frac{i\,e^{ix\sin\theta_0}}{\pi}\sum_{m=1}^{n} \frac{(-1)^{m-1}2^{2m}(n+m-1)!}{\Delta^{2m}(2m-1)!(n-m)!}\Phi(e^{ix/\Delta}, 1-2m, \Delta\sin\theta_0). \tag{3.38}$$

For odd order series $S_{2n+1}^H(x)$, similar pleasing simplifications are in place after the substitution of the obtained expression for $F_{2n+1}(x)$ (3.37) and the corresponding integrals (A 8) and (A 10) into (3.18). The double sums of integral (A 8) cancel the double sums of the Coates integral (A 10) and the Neumann function of the closed-form expression of the Coates integral (A 10) cancels the last term of (3.18). The first two terms of $F_{2n+1}(x)$ (3.37) cancel the single sum of integral (A 8) and the expression for $S_{2n+1}^H(x)$ takes the final form

$$S_{2n+1}^H(x) = 2\sum_{p=-\infty}^{-1} \frac{e^{i(2n+1)\theta_p + ix\sin\theta_p}}{D\cos\theta_p} - 2\sum_{p=0}^{\infty} \frac{e^{-i(2n+1)\theta_p + ix\sin\theta_p}}{D\cos\theta_p} + \frac{2}{\pi\Delta}\frac{e^{ix\sin\theta_0}}{1-e^{ix/\Delta}} + \frac{2\,e^{ix\sin\theta_0}}{\pi}\sum_{m=1}^{n} \frac{(-1)^m 2^{2m}(n+m)!}{(2m)!(n-m)!\Delta^{2m+1}}\Phi(e^{ix/\Delta}, -2m, \Delta\sin\theta_0). \tag{3.39}$$

Therefore, the Schlömilch series (1.1) involving Hankel functions can be expressed in terms of an absolutely converging series of elementary functions and a finite sum involving Lerch transcendent functions. The obtained expression (3.39) can be rewritten in a more compact form by incorporating the third term into the finite sum given the relation

$$\Phi(e^{ix/\Delta}, 0, \Delta\sin\theta_0) = \frac{1}{1-e^{ix/\Delta}}, \tag{3.40}$$

which is applicable if $\theta_0 \neq 0$. Hence the series (3.39) can be rewritten as

$$S_{2n+1}^H(x) = 2\sum_{p=-\infty}^{-1} \frac{e^{i(2n+1)\theta_p + ix\sin\theta_p}}{D\cos\theta_p} - 2\sum_{p=0}^{\infty} \frac{e^{-i(2n+1)\theta_p + ix\sin\theta_p}}{D\cos\theta_p} + \frac{e^{ix\sin\theta_0}}{\pi}\sum_{m=0}^{n} \frac{(-1)^m 2^{2m+1}(n+m)!}{(2m)!(n-m)!\Delta^{2m+1}}\Phi(e^{ix/\Delta}, -2m, \Delta\sin\theta_0). \tag{3.41}$$

Note that the series for $S_1^H(x)$ is represented in terms of elementary functions only as it is given by the first three terms of equation (3.39). For the particular value of $x = D/2$, the Lerch transcendent functions in equations (3.38) and (3.41) reduce to Euler polynomials [2] given the connection $E_m(x) = 2\Phi(-1, -m, x)$. Therefore, for this case also the Schlömilch series involving Hankel functions are represented in terms of elementary functions only. Given the rich properties of the Lerch transcendent function there are other interesting argument values where $S_n^H(x)$ can be expressed in terms of elementary functions only; however, we will not pursue this here. Expressions (3.38) and (3.41) are the key findings of this paper.

It is worthwhile mentioning that the Lerch transcendent function in (3.38) and (3.41) is also called the Lerch zeta function, denoted by $L(x/D, s, \alpha)$ provided the following relation $\Phi(e^{i2\pi x/D}, s, \alpha) = L(x/D, s, \alpha)$. In §6, the accuracy, efficiency and the numerical verification of the derived summation formulae (3.38) and (3.41) will be demonstrated.

4. The summation formulae for the $S_n^J(x)$ and $S_n^Y(x)$ series

In this section, we provide details of the derivation of the summation formulae for the $S_n^J(x)$ and $S_n^Y(x)$ series. The summation equation for the $S_n^Y(x)$ series can be derived using a similar approach to that for the $S_n^H(x)$ series. However, it is easier first to derive the summation formula for the $S_n^J(x)$ series, which does not require a limiting process, and then to deduce the summation formula for $S_n^Y(x)$ by using the relation $S_n^Y(x) = (S_n^H(x) - S_n^J(x))/i$ between the series.

The Bessel series for $S_n^J(x)$ has the form

$$S_n^J(x) = \sum_{s=-\infty}^{\infty} J_n(|sD - x|)\,\mathrm{e}^{-in\arg(sD-x)}\,\mathrm{e}^{\mathrm{i}sD\sin\theta_0}. \tag{4.1}$$

The integral representation for the Bessel function can be written as

$$J_n(|sD - x|)\,\mathrm{e}^{-\mathrm{i}n\arg(sD-x)} = \frac{1}{2\pi}\int_{-1}^{1}\left(\left[\sqrt{1-t^2}-\mathrm{i}t\right]^n + (-1)^n\left[\sqrt{1-t^2}+\mathrm{i}t\right]^n\right)\frac{\mathrm{e}^{\mathrm{i}(sD-x)t}}{\sqrt{1-t^2}}\,\mathrm{d}t. \tag{4.2}$$

Note that the integration in (4.2) is carried out over the propagating part of the spectrum only, $|t| < 1$. Now we substitute (4.2) into (4.1) then interchange the integration and summation, and, using either the Poisson summation formula (2.8) or the identity (2.9), the expression for $S_n^J(x)$ takes the form

$$S_n^J(x) = \frac{1}{D}\sum_{p=-p_-}^{p_+}\left(\mathrm{e}^{in\theta_p} + (-1)^n\,\mathrm{e}^{-\mathrm{i}n\theta_p}\right)\frac{\mathrm{e}^{\mathrm{i}x\sin\theta_p}}{\cos\theta_p}. \tag{4.3}$$

From the obtained relation (4.3), it is easy to deduce the series expressions for even and odd n order cases. For the even case, we deduce

$$S_{2n}^J(x) = \frac{2}{D}\sum_{p=-p_-}^{p_+}\frac{\cos 2n\theta_p}{\cos\theta_p}\,\mathrm{e}^{\mathrm{i}x\sin\theta_p}, \tag{4.4}$$

while for the odd case the formula takes the form

$$S_{2n+1}^J(x) = \frac{2\mathrm{i}}{D}\sum_{p=-p_-}^{p_+}\frac{\sin(2n+1)\theta_p}{\cos\theta_p}\,\mathrm{e}^{\mathrm{i}x\sin\theta_p}. \tag{4.5}$$

Note that the summation in (4.4) and (4.5) is carried out only over propagating plane waves orders $|\sin\theta_p| < 1$. The obtained result for the even case (4.4) coincides with the result reported in [2]. This can be seen after a straightforward change in nomenclature and given that $\cos 2n\theta_p$ can be expressed in terms of the Chebyshev polynomials of the first kind $T_n(x)$ using the following connection $\cos 2n\theta_p = (-1)^n T_{2n}(\sin\theta_p)$, where

$$T_n(x) = \frac{1}{2}\left[(x+\mathrm{i}\sqrt{1-x^2})^n + (x-\mathrm{i}\sqrt{1-x^2})^n\right]. \tag{4.6}$$

Therefore, in terms of the Chebyshev polynomials the even order series (4.1) takes the form

$$S_{2n}^J(x) = \frac{2(-1)^n}{D}\sum_{p=-p_-}^{p_+}\frac{T_{2n}(\sin\theta_p)}{\cos\theta_p}\,\mathrm{e}^{\mathrm{i}x\sin\theta_p}. \tag{4.7}$$

Similarly, the odd order series (4.1) can be expressed in terms of the odd order Chebyshev polynomials

$$S_{2n+1}^J(x) = \frac{2\mathrm{i}(-1)^n}{D}\sum_{p=-p_-}^{p_+}\frac{T_{2n+1}(\sin\theta_p)}{\cos\theta_p}\,\mathrm{e}^{\mathrm{i}x\sin\theta_p}. \tag{4.8}$$

The expressions for the even order sum (4.4) or (4.7) are applicable for the zero order sum $S_0^J(x)$ also, which can be written as

$$S_0^J(x) = \frac{2}{D} \sum_{p=-p_-}^{p_+} \frac{e^{ix\sin\theta_p}}{\cos\theta_p}. \tag{4.9}$$

The expressions for the $S_n^Y(x)$ series can now be readily deduced by subtracting the obtained expressions for the series $S_n^J(x)$, (4.4) and (4.5), from the corresponding series for $S_n^H(x)$, (3.38) and (3.41). After some straightforward algebraic transformations, the formula for the $S_{2n}^Y(x)$ series takes the form

$$\begin{aligned} S_{2n}^Y(x) &= \frac{2}{D}\left(\sum_{p=-p_-}^{-1} - \sum_{p=0}^{p_+}\right)\frac{\sin 2n\theta_p}{\cos\theta_p}\,e^{ix\sin\theta_p} \\ &\quad - \frac{2(-1)^n}{D}\left(\sum_{p=p_-+1}^{\infty}\frac{e^{-2n\eta_p^- - ix\cosh\eta_p^-}}{\sinh\eta_p^-} + \sum_{p=p_++1}^{\infty}\frac{e^{-2n\eta_p^+ + ix\cosh\eta_p^+}}{\sinh\eta_p^+}\right) \\ &\quad + \frac{e^{ix\sin\theta_0}}{\pi}\sum_{m=1}^{n}\frac{(-1)^{m-1}2^{2m}(n+m-1)!}{\Delta^{2m}(2m-1)!(n-m)!}\,\Phi(e^{ix/\Delta}, 1-2m, \Delta\sin\theta_0), \end{aligned} \tag{4.10}$$

where

$$\cosh\eta_p^{\pm} = \frac{2\pi p}{D} \pm \sin\theta_0, \tag{4.11}$$

while the odd order series $S_{2n+1}^Y(x)$ can be expressed as

$$\begin{aligned} S_{2n+1}^Y(x) &= \frac{2i}{D}\left(\sum_{p=0}^{p_+} - \sum_{p=-p_-}^{-1}\right)\frac{\cos(2n+1)\theta_p}{\cos\theta_p}\,e^{ix\sin\theta_p} \\ &\quad - \frac{2i(-1)^n}{D}\left(\sum_{p=p_++1}^{\infty}\frac{e^{-(2n+1)\eta_p^+ + ix\cosh\eta_p^+}}{\sinh\eta_p^+} - \sum_{p=p_-+1}^{\infty}\frac{e^{-(2n+1)\eta_p^- - ix\cosh\eta_p^-}}{\sinh\eta_p^-}\right) \\ &\quad - \frac{i\,e^{ix\sin\theta_0}}{\pi}\sum_{m=0}^{n}\frac{(-1)^m 2^{2m+1}(n+m)!}{(2m)!(n-m)!\Delta^{2m+1}}\,\Phi(e^{ix/\Delta}, -2m, \Delta\sin\theta_0). \end{aligned} \tag{4.12}$$

For completeness, we provide the expression for the series $S_0^Y(x)$, which can be obtained either by using the relations (2.15) and (4.9)

$$S_0^Y(x) = -\frac{2}{D}\left(\sum_{p=p_-+1}^{\infty}\frac{e^{-ix\cosh\eta_p^-}}{\sinh\eta_p^-} + \sum_{p=p_++1}^{\infty}\frac{e^{ix\cosh\eta_p^+}}{\sinh\eta_p^+}\right) \tag{4.13}$$

or directly through equation (4.10), where the last term is dropped and the value for n is replaced by zero throughout.

5. Series $S_n^Z(x)$ for $\theta_0 = 0$

In this section, we consider the Schlömilch series (1.1) for $\theta_0 = 0$. These series arise in the case of a plane wave incidence normal to the surface of a grating. As the incidence angle vanishes $\theta_0 = 0$, for the normal incidence the initial Schlömilch series takes the form

$$S_n^Z(x) = \sum_{s=-\infty}^{\infty} Z_n(|sD - x|)\,e^{-in\arg(sD-x)}. \tag{5.1}$$

The formulae for the normal incidence can be readily deduced from the corresponding general formulae for off-axis incidence by taking the limit $\theta_0 \to 0$. In this case, there is a symmetry between the positive and negative diffraction orders

$$\sin\theta_p = \frac{p}{\Delta} = -\sin\theta_{-p} \tag{5.2}$$

and we also have $p_- = p_+ = [\Delta] = [m_\pm]$, where $p_\pm$ are the largest integer smaller than $m_\pm$. For the case of the Schlömilch series involving Hankel functions $S_n^H(x)$, the Lerch transcendent function reduces to Jonquière's function [2], which is more commonly known as the polylogarithm function $Li_s(z)$ [31]

$$\lim_{\theta_0\to 0} \Phi(\mathrm{e}^{\mathrm{i}x/\Delta}, 1-2m, \Delta\sin\theta_0) = Li_{1-2m}(\mathrm{e}^{\mathrm{i}x/\Delta}), \tag{5.3}$$

where $Li_s(z)$ is defined by

$$Li_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s}. \tag{5.4}$$

Therefore, by using the symmetries between the diffraction orders (5.2), the even order Schlömilch series involving the Hankel functions (3.38) takes the form

$$S_{2n}^H(x) = \frac{2}{D} + \frac{4}{D}\sum_{p=1}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}2n\theta_p}\cos(x\sin\theta_p)}{\cos\theta_p} + \frac{\mathrm{i}}{\pi}\sum_{m=1}^{n} \frac{(-1)^{m-1}2^{2m}(n+m-1)!}{\Delta^{2m}(2m-1)!(n-m)!} Li_{1-2m}(\mathrm{e}^{\mathrm{i}x/\Delta}), \tag{5.5}$$

while the odd order series (3.39) reduces to

$$\begin{aligned} S_{2n+1}^H(x) = {} & \frac{\mathrm{i}}{\pi\Delta}\cot\frac{x}{2\Delta} - \frac{4\mathrm{i}}{D}\sum_{p=1}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(2n+1)\theta_p}\sin(x\sin\theta_p)}{\cos\theta_p} \\ & + \frac{1}{\pi}\sum_{m=1}^{n} \frac{(-1)^m 2^{2m+1}(n+m)!}{\Delta^{2m+1}(2m)!(n-m)!} Li_{-2m}(\mathrm{e}^{\mathrm{i}x/\Delta}). \end{aligned} \tag{5.6}$$

The expression for the odd order series (5.6) can also be written as

$$S_{2n+1}^H(x) = \frac{1}{\pi\Delta} - \frac{4\mathrm{i}}{D}\sum_{p=1}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(2n+1)\theta_p}\sin(x\sin\theta_p)}{\cos\theta_p} + \frac{1}{\pi}\sum_{m=0}^{n} \frac{(-1)^m 2^{2m+1}(n+m)!}{\Delta^{2m+1}(2m)!(n-m)!} Li_{-2m}(\mathrm{e}^{\mathrm{i}x/\Delta}), \tag{5.7}$$

given the relation for the zero order of the polylogarithm function

$$Li_0(\mathrm{e}^{\mathrm{i}x/\Delta}) = \frac{e^{ix/\Delta}}{1-\mathrm{e}^{\mathrm{i}x/\Delta}}. \tag{5.8}$$

Relation (5.5) can be used to derive the summation equation for the series $S_0^H(x)$ for normal incidence. The summation equation for $S_0^H(x)$ is obtained by substituting $n=0$ in (5.5) and dropping the last term to obtain

$$S_0^H(x) = \frac{2}{D} + \frac{4}{D}\sum_{p=1}^{\infty} \frac{\cos(x\sin\theta_p)}{D\cos\theta_p}. \tag{5.9}$$

The expressions for the summation equations for the Schlömilch series for $\theta_0 = 0$ involving Bessel functions $S_n^J(x)$ are readily deduced from equations (4.4) and (4.5). The expression for the even order series $S^J_{2n}(x)$ takes the form

$$S^J_{2n}(x) = \frac{2}{D} + \frac{4}{D}\sum_{p=1}^{p_+}\frac{\cos 2n\theta_p}{\cos\theta_p}\cos(x\sin\theta_p), \tag{5.10}$$

while the expression for the odd order series $S^J_{2n+1}(x)$ can be written as

$$S^J_{2n+1}(x) = -\frac{4}{D}\sum_{p=1}^{p_+}\frac{\sin(2n+1)\theta_p}{\cos\theta_p}\sin(x\sin\theta_p). \tag{5.11}$$

The Neumann series for the normal incidence can be obtained using results (5.5) and (5.10) for the even order case and relations (5.6) and (5.11) for odd series or by taking the limit $\theta_0 \to 0$ in (4.10) and (4.12). The summation formulae for the Schlömilch series for $\theta_0 = 0$ involving the Neumann series take the forms

$$\begin{aligned} S^Y_{2n}(x) = &-\frac{4}{D}\sum_{p=1}^{p_+}\frac{\sin 2n\theta_p\cos(x\sin\theta_p)}{\cos\theta_p} - \frac{4(-1)^n}{D}\sum_{p=p_++1}^{\infty}\frac{\mathrm{e}^{-2n\eta_p^+}\cos(x\cosh\eta_p^+)}{\sinh\eta_p^+} \\ &+\frac{1}{\pi}\sum_{m=1}^{n}\frac{(-1)^{m-1}2^{2m}(n+m-1)!}{\Delta^{2m}(2m-1)!(n-m)!}Li_{1-2m}(\mathrm{e}^{\mathrm{i}x/\Delta}) \end{aligned} \tag{5.12}$$

and

$$\begin{aligned} S^Y_{2n+1}(x) = &\frac{1}{\pi\Delta}\cot\frac{x}{2\Delta} - \frac{4}{D}\sum_{p=1}^{p_+}\frac{\cos(2n+1)\theta_p\sin(x\sin\theta_p)}{\cos\theta_p} \\ &+\frac{4(-1)^n}{D}\sum_{p=p_++1}^{\infty}\frac{\mathrm{e}^{-(2n+1)\eta_p^+}\sin(x\cosh\eta_p^+)}{\sinh\eta_p^+} - \frac{\mathrm{i}}{\pi}\sum_{m=1}^{n}\frac{(-1)^m 2^{2m+1}(n+m)!}{\Delta^{2m+1}(2m)!(n-m)!}Li_{-2m}(\mathrm{e}^{\mathrm{i}x/\Delta}) \end{aligned} \tag{5.13}$$

for the even and odd orders, respectively.

6. Numerical verification

Apart from the considerable theoretical interest of the presented results, the obtained expressions for the Schlömilch series are important for applications also. In this section, we provide details of the numerical verifications for the derived analytical expressions (3.38) and (3.41) for the Schlömilch series $S^H_n(x)$ as well as for the series $S^J_n(x)$ and show their accuracy and efficiency.

In applications, the numerical values for $S^Z_n(x)$ must be obtained with an accuracy of at least seven significant figures, which is quite challenging for large values of the period $D \gg 1$. At the same time, larger values of D are required either for the modelling of wave propagation in photonic or phononic crystals with embedded intricate structures [9,10] or for investigating the fundamental phenomenon of Anderson localization of classical waves [17–19].

The analytical expressions (3.38) and (3.41) are ideally suited for numerical calculations. Indeed, the obtained expressions involve the absolutely converging series of elementary functions and Lerch transcendent functions which can be calculated with high precision. The rate of convergence of the elementary series $S^H_n(x)$ for even order (3.38) is $p^{-(2n+1)}$, where p is the summation index of the series. Therefore, the slowest convergence rate for the even order series occurs for $S^H_2(x)$, which converges as p^{-3}. The rate of convergence for odd order series $S^H_{2n+1}(x)$ is $p^{-(2n+2)}$. So the slowest convergence rate for odd order series occurs for $S^H_1(x)$, which converges as p^{-2}. If required, the convergence rate can be accelerated further using Kummer's transformation [16,27,28]. Note that the convergence rate increases substantially with the increase in the series order n.

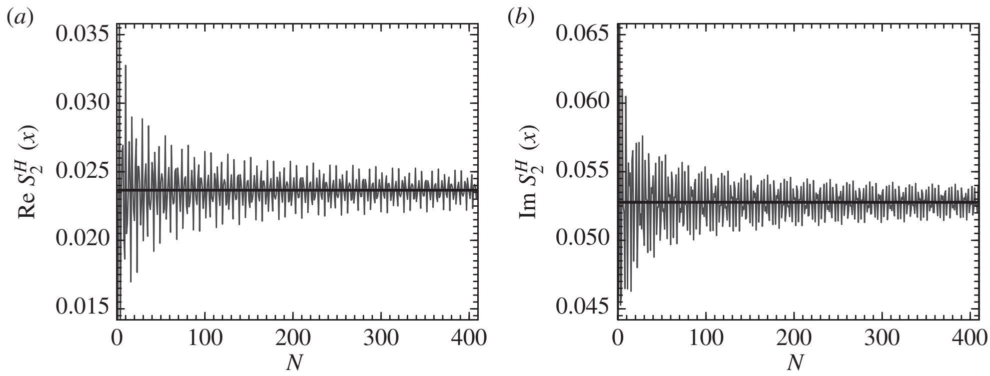

Figure 1. The real part of the partial sum of $S_2^H(250)$ (*a*) and the imaginary part of the partial sum of $S_2^H(250)$ (*b*) (oscillating line); the straight line is the value for the series calculated based on the derived analytical result (3.38). The label of the horizontal axis N represents the order of the partial sum of the initial series (1.1).

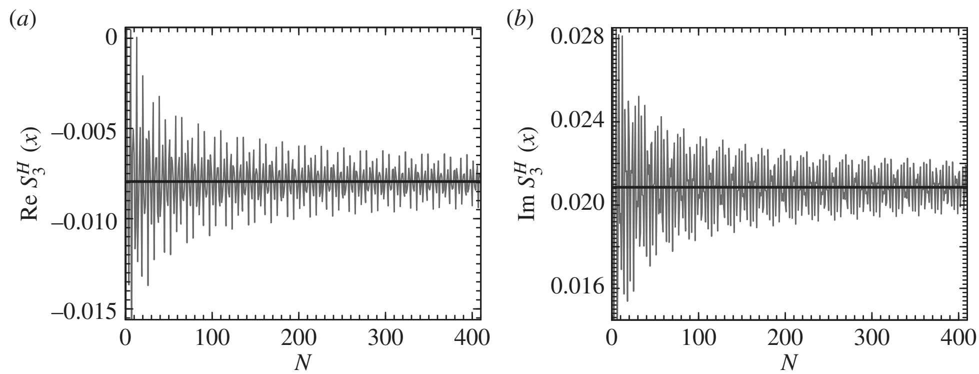

Figure 2. The same relationship as in figure 1 but for the series $S_3^H(250)$. The straight line is the value for the series calculated using the derived analytical result (3.41).

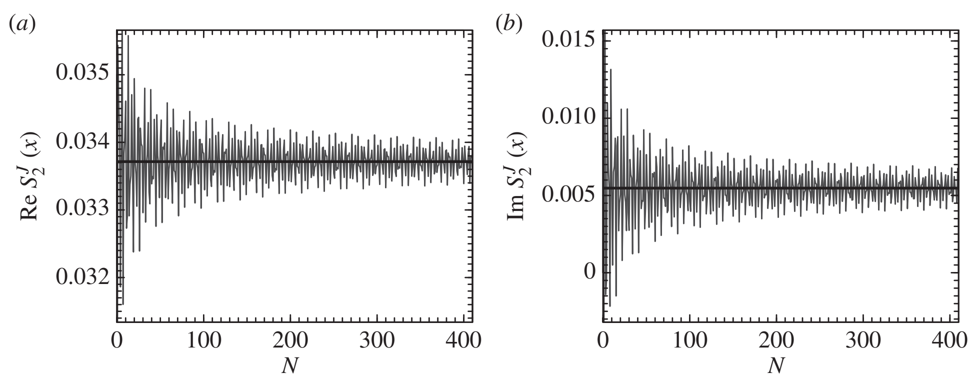

Figure 3. The same relationship as in figure 1 but for the series $S_2^J(250)$. The straight line is the value for the series calculated using the derived analytical result (4.4).

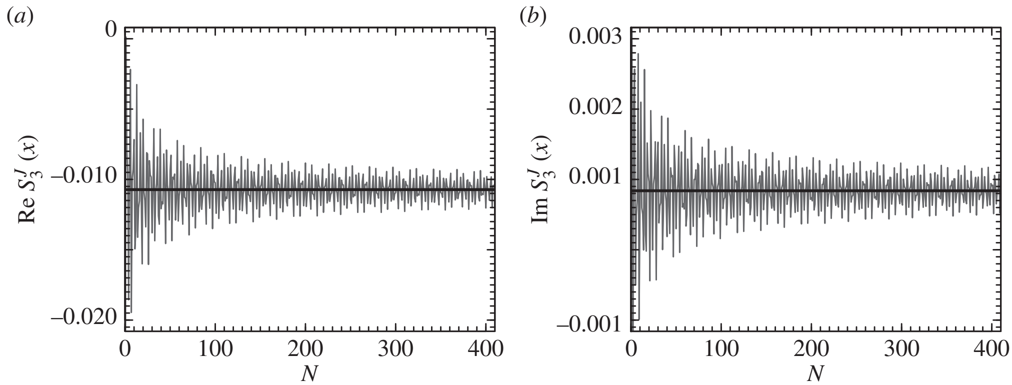

Figure 4. The same relationship as in figure 1 but for the series $S_3^J(250)$. The straight line is the value for the series calculated using the derived analytical result (4.5).

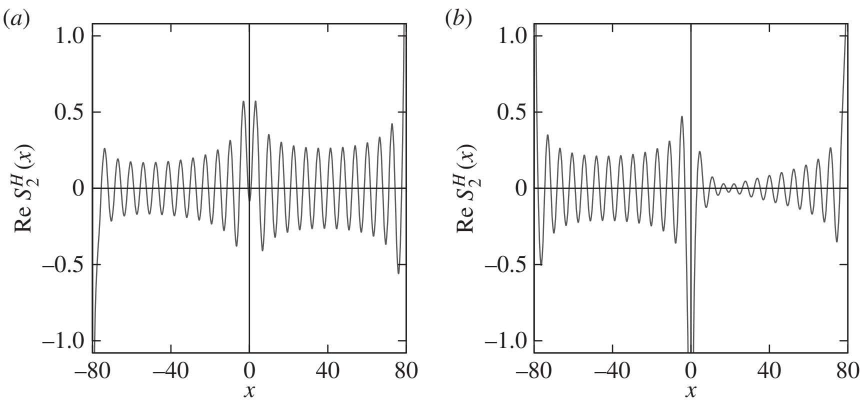

Figure 5. The real (a) and imaginary (b) parts of $S_2^H(x)$ as a function of x for $D = 80$ and $\theta_0 = \pi/6$.

First, the consistency between the obtained equations (3.38), (3.41) and the relation (1.3) has been verified. In table 1, we present the comparison data for the values $S_2^H(x)$ and $S_3^H(x)$ for the following input set of the parameters: $D = 80$, $\theta_0 = \pi/6$ and $x = 79$. There is an excellent agreement between the computed values. The values calculated based on (3.38) and (3.41) are correct with all presented figures. The values based on the relation (1.3) have been calculated with 160 terms, which requires calculation of series (1.2) for up to 80 orders of $\tilde{S}_n$. The input parameters used in the calculations for $S_n^H(x)$ in table 1 are the typical parameters considered for the modelling of scattering problems on gratings or photonic crystals. These parameters correspond to modelling of gratings with $N \approx 30$ inclusions per unit cell for typical wavelengths. The obtained expressions for the Schlömilch series (3.38) and (3.41) enable the modelling of structures with substantially larger unit cells, thus allowing a substantial increase in the number of inclusions per unit cell. In figure 1, we plot the partial sums of the series $S_2^H(x)$ for the input parameters $D = 1000$, $\theta_0 = \pi/6$ and $x = 250$. The oscillating curves in figure 1*a*,*b* are the real and imaginary parts of the partial sums of the series $S_2^H(250)$, respectively, while the straight lines are the values for $S_2^H(250)$ calculated using the analytical result (3.38). In figure 2, we plot the same relationship as in figure 1 but for the series $S_3^H(250)$. It is clear from these plots that the series $S_n^H(x)$ are very slowly converging series, which makes the accurate calculations of (1.1) by direct summation useless, while the obtained analytical expressions for the series (3.38) and (3.41) are very accurate and efficient. In figures 3 and 4, we plot the same relationship as in figure 1 but for the series $S_2^J(250)$

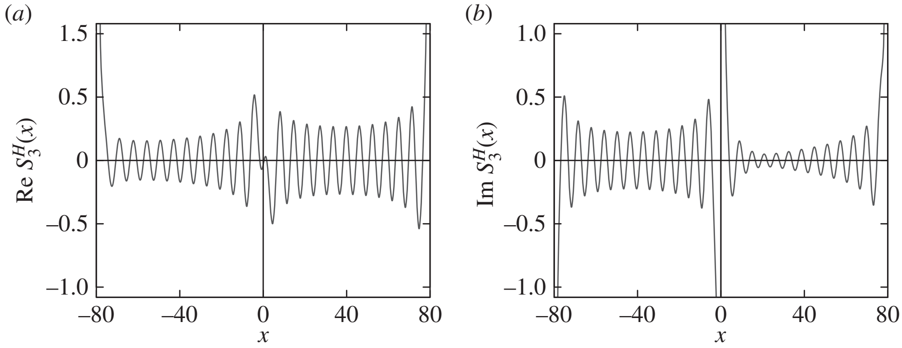

Figure 6. The same relationship as in figure 5 but for $S_3^H(x)$.

Table 1. A comparison between the numerical values for $S_2^H(79)$ and $S_3^H(79)$ calculated using the derived analytical equations (3.38), (3.41) (the second row in the table) and using equation (1.3) (the first row in the table).

	$n = 2$	$n = 3$
equation (1.3)	$1.2967512057 + i1.2880578695$	$4.4255742913 + i3.8727633391$
equations (3.38), (3.41)	$1.2967512010 + i1.2880578655$	$4.4255742886 + i3.8727633367$

and $S_3^J(250)$. The straight lines passing through the oscillating curves of the partial sums for the corresponding series for $S_n^J(x)$ have been calculated using relations (4.4) and (4.5), respectively. These plots along the comparison data presented in table 1 verify the validity, accuracy and efficiency of the obtained analytical expressions for the series $S_n^Z(x)$.

The summation equations for the series $S_n^Z(x)$ have also been verified for the normal incidence case $\theta_0 = 0$. The plots of the partial sums of $S_n^Z(x)$ are similar to those for the considered cases above for $\theta_0 = \pi/6$ and they are not provided here. The obtained summation formulae (3.38) and (3.41) satisfy analytically the quasi-periodicity conditions (2.2) and (2.3). These conditions have also been verified numerically.

Given the obtained series (3.38) and (3.41) converge absolutely, the number of significant figures that can be achieved is only limited by the standard function accuracy and limits set by a computer. The presented calculations have been done using Wolfram Mathematica [32] with double precision accuracy. The computational time is of the same order as for the calculation of the series (1.2) based on the Twersky formulae [13].

Having verified numerically the accuracy and efficiency of the obtained summation formulae, it is interesting to plot $S_n^Z(x)$ as a function of x. In figure 5, we plot $S_2^H(x)$ as a function of x for $\theta_0 = \pi/6$, $D = 80$ in the domain $-D < x < D$. The real part of $S_2^H(x)$ is plotted in figure 5*a*, whereas the imaginary part is plotted in figure 5*b*. Both the real and imaginary parts of $S_2^H(x)$ are oscillatory functions of x. The real part of $S_2^H(x)$ is continuous at $x = 0$, whereas the imaginary part diverges. Both the real and imaginary parts of $S_2^H(x)$ diverge at $x = \pm D$.

In figure 6, we plot the same relationship as in figure 5 but for the series $S_3^H(x)$. The overall behaviour of $S_3^H(x)$ is quite similar to $S_2^H(x)$. In contrast with $S_2^H(x)$, the real part of $S_3^H(x)$ passes through the origin. As the period D increases the oscillatory behaviour of $S_n^H(x)$ also increases. The behaviours of the $S_n^Y(x)$ and $S_n^J(x)$ series are quite similar to that of $S_n^H(x)$ except $S_n^J(x)$ is a continuous function of x and we do not provide their plots here.

7. Conclusion

Accurate and efficient summation equations for the Schlömilch type series (1.1) have been derived. This is achieved by using the Euler summation formula in the form given by Nörlund [14]. The obtained analytical formulae (3.38) and (3.41) for the Schlömilch series involving the

Hankel functions or Neumann functions are expressed in terms of an absolutely convergent series of elementary functions and a finite sum of Lerch transcendent functions. The obtained equations have been verified numerically and their accuracy and efficiency have been demonstrated. The summation equations for the Schlömilch series involving the Bessel functions are expressed in terms of a finite sum of elementary functions only (equations (4.4) and (4.5)).

The summation equations for the Schlömilch series at the normal incidence $\theta_0 = 0$ have also been derived (equations (5.10)–(5.13)). For the Schlömilch series involving the Hankel functions or Neumann functions, the summation formulae are expressed in terms of an absolutely convergent series of elementary functions and a finite sum of polylogarithm functions. The closed-form expressions for the Coates integrals [21], required for the derivation of the summation equations, have been obtained (see equations (A 9), (A 10) and the electronic supplementary material). These analytical expressions for the Coates integrals have been verified numerically.

The obtained results, apart from their considerable analytical importance, also allow the modelling of scattering problems with substantially larger unit cells. Therefore, the presented results permit accurate and efficient modelling of extended devices embedded in photonic crystals, or characterization of the transmission properties of phononic crystals. The effects of manufacturing imperfections on their functional properties can also be investigated. The obtained results are also important for the accurate characterization of the phenomenon of Anderson localization of classical waves [17–19], where the ability to consider substantially larger unit cells is essential.

Therefore, the derived analytical formulae presented here complement the results by von Ignatovsky [11,12] and Twersky [13] and extend the available analytical toolbox for modelling a variety of important and exciting fundamental and applied problems in physics.

Data accessibility. The data used here have been produced using the obtained equations.
Competing interests. I have no competing interests.
Funding. I received no funding for this study.
Acknowledgements. The computational resources used in this work were provided by Intersect Ltd. The unequivocal support and encouragement from my family and the full understanding of my wife (most of the time) is gratefully acknowledged.

Appendix A. Closed form of integrals over the finite interval in equations (3.15) and (3.18)

Here we provide details for the calculation of integrals over the finite region appearing in (3.15) and (3.18). To find the closed-form expression for the integral

$$\int_0^{\pi/2} \cos(x \sin\theta_p) \sin(2n\theta_p)\, \mathrm{d}\theta_p, \tag{A 1}$$

we first multiply and divide the integrand of (A 1) by $\cos\theta_p$ and use relation (3.22). After the substitution $t = x \sin\theta_p$, the initial integral (A 1) can be expressed as

$$\int_0^{\pi/2} \cos(x \sin\theta_p) \sin(2n\theta_p)\, \mathrm{d}\theta_p = \sum_{m=1}^{n} \frac{(-1)^{m-1} 2^{2m-1} (n+m-1)!}{(2m-1)!(n-m)! x^{2m}} \int_0^x t^{2m-1} \cos t\, \mathrm{d}t. \tag{A 2}$$

This integral can be calculated in closed form by using the standard result [30]

$$\int_0^x t^{2m-1} \cos t\, \mathrm{d}t = (2m-1)! \left[\sum_{k=0}^{m-1} \frac{(-1)^k x^{2m-2k-1} \sin x}{(2m-2k-1)!} + \sum_{k=0}^{m-1} \frac{(-1)^k x^{2m-2k-2} \cos x}{(2m-2k-2)!} - (-1)^{m-1} \right]. \tag{A 3}$$

The final form for the integral (A 1) takes the form

$$\begin{aligned}\int_0^{\pi/2}\cos(x\sin\theta_p)\sin(2n\theta_p)\,\mathrm{d}\theta_p &= \sum_{m=1}^{n}\frac{(-1)^{m-1}2^{2m-1}(n+m-1)!}{(n-m)!}\sum_{k=0}^{m-1}\frac{(-1)^k\sin x}{x^{2k+1}(2m-2k-1)!}\\ &\quad+\sum_{m=1}^{n}\frac{(-1)^{m-1}2^{2m-1}(n+m-1)!}{(n-m)!}\sum_{k=0}^{m-1}\frac{(-1)^k\cos x}{x^{2k+2}(2m-2k-2)!}\\ &\quad-\sum_{m=1}^{n}\frac{2^{2m-1}(n+m-1)!}{x^{2m}(n-m)!}.\end{aligned}\tag{A 4}$$

The finding of the closed-form expression for the integral

$$\int_0^{\pi/2}\sin(x\sin\theta_p)\cos(2n+1)\theta_p\,\mathrm{d}\theta_p \tag{A 5}$$

is quite similar to integral (A 1). We first multiply and divide the integrand of (A 5) by $\cos\theta_p$ and apply identity (3.33). Now we use the substitution $t=x\sin\theta_p$ and express (A 5) as

$$\int_0^{\pi/2}\sin(x\sin\theta_p)\cos(2n+1)\theta_p\,\mathrm{d}\theta_p=\sum_{m=0}^{n}\frac{(-1)^m2^{2m}(n+m)!}{(2m)!(n-m)!x^{2m+1}}\int_0^x t^{2m}\sin t\,\mathrm{d}t. \tag{A 6}$$

The obtained integral can be calculated using the standard result [30]

$$\int_0^x t^{2m}\sin t\,\mathrm{d}t=(2m)!\left[\sum_{k=0}^{m}\frac{(-1)^k x^{2m-2k-1}\sin x}{(2m-2k-1)!}+\sum_{k=0}^{m}\frac{(-1)^{(k+1)}x^{2m-2k}\cos x}{(2m-2k)!}-(-1)^{m-1}\right]. \tag{A 7}$$

After the substitution of (A 7) into (A 6), the closed form of (A 5) takes the form

$$\begin{aligned}\int_0^{\pi/2}\sin(x\sin\theta_p)\cos(2n+1)\theta_p\mathrm{d}\theta_p &= \sum_{m=0}^{n}\frac{(-1)^m2^{2m}(n+m)!}{(n-m)!}\sum_{k=0}^{m}\frac{(-1)^{(k+1)}\cos x}{x^{2k+1}(2m-2k)!}\\ &\quad+\sum_{m=1}^{n}\frac{(-1)^m2^{2m}(n+m)!}{(n-m)!}\sum_{k=0}^{m-1}\frac{(-1)^k\sin x}{x^{2k+2}(2m-2k-1)!}\\ &\quad+\sum_{m=0}^{n}\frac{2^{2m}(n+m)!}{x^{2m+1}(n-m)!}.\end{aligned}\tag{A 8}$$

The obtained closed-form expressions of (A 4) and (A 8) have also been verified numerically for different input parameters x and n.

The closed-form expressions for the Coates's integrals are given by the relations

$$\begin{aligned}I_{2n}=\int_0^\infty\cos(x\cosh t)\,\mathrm{e}^{-2nt}\,\mathrm{d}t &= (-1)^{n+1}\left[\frac{\pi}{2}Y_{2n}(|x|)+\sum_{m=1}^{n}\frac{(-1)^{m-1}2^{2m-1}(n+m-1)!}{(n-m)!}\right.\\ &\quad\left.\times\sum_{k=0}^{m-1}\frac{(-1)^k\sin x}{x^{2k+1}(2m-2k-1)!}+\sum_{m=1}^{n}\frac{(-1)^{m-1}2^{2m-1}(n+m-1)!}{(n-m)!}\sum_{k=0}^{m-1}\frac{(-1)^k\cos x}{x^{2k+2}(2m-2k-2)!}\right]\end{aligned}\tag{A 9}$$

and

$$\begin{aligned}I_{2n+1}=\int_0^\infty\sin(x\cosh t)\,\mathrm{e}^{-(2n+1)t}\,\mathrm{d}t &= (-1)^{n+1}\left[\frac{\pi}{2}Y_{2n+1}(|x|)\,\mathrm{e}^{\mathrm{i}(2n+1)\arg(x)}-\sum_{m=0}^{n}\frac{(-1)^m2^{2m}(n+m)!}{(n-m)!}\right.\\ &\quad\left.\times\sum_{k=0}^{m}\frac{(-1)^{k+1}\cos x}{x^{2k+1}(2m-2k)!}-\sum_{m=1}^{n}\frac{(-1)^m2^{2m}(n+m)!}{(n-m)!}\sum_{k=0}^{m-1}\frac{(-1)^k\sin x}{x^{2k+2}(2m-2k-1)!}\right].\end{aligned}\tag{A 10}$$

Their derivation is given in the electronic supplementary material.

References

1. Watson GN. 1966 *A treatise on the theory of Bessel functions*. Cambridge, UK: Cambridge University Press.
2. Magnus W, Oberhettinger F, Soni PR. 1966 *Formulas and theorems for the special functions of mathematical physics*, p. 133. New York, NY: Springer.
3. Botten LC, Nicorovici NA, Asatryan AA, McPhedran RC, de Sterke CM, Robinson PA. 2000 Formulation for electromagnetic scattering and propagation through grating stacks of metallic and dielectric cylinders for photonic crystal calculations. Part I. Method. *J. Opt. Soc. Am. A* **17**, 2165–2176. (doi:10.1364/JOSAA.17.002165)
4. Botten LC, Nicorovici NA, Asatryan AA, McPhedran RC, de Sterke CM, Robinson PA. 2000 Formulation for electromagnetic scattering and propagation through grating stacks of metallic and dielectric cylinders for photonic crystal calculations. Part II. Method. *J. Opt. Soc. Am. A* **17**, 2177–2190. (doi:10.1364/JOSAA.17.002177)
5. Hutley M. 1982 *Diffraction gratings* (*techniques of physics*). New York, NY: Academic Press.
6. Joannopoulos JD, Johnson SG, Winn JN, Meade RD. 2008 *Photonic crystals: molding the flow of light*. Princeton, NJ: Princeton University Press.
7. Marcos P, Soukoulis CM. 2008 *Wave propagation from electrons to photonic crystals and left-handed materials*. Princeton, NJ: Princeton University Press.
8. Sigalas MM, Economou EN. 1992 Elastic and acoustic wave band structure. *J. Sound Vib.* **158**, 377–382. (doi:10.1016/0022-460X(92)90059-7)
9. Botten LC, Asatryan AA, Langtry TN, White TP, de Sterke CM, McPhedran RC. 2003 Semianalytic treatment for propagation in finite photonic crystal waveguides. *Opt. Lett.* **28**, 854–856. (doi:10.1364/OL.28.000854)
10. Langtry TN, Asatryan AA, Botten LC, de Sterke CM, McPhedran RC, Robinson PA. 2003 Effects of disorder in two-dimensional photonic crystal waveguides. *Phys. Rev. E* **68**, 026611. (doi:10.1103/PhysRevE.68.026611)
11. von Ignatovsky W. 1913 Über Reihen mit Zylinderfunctionen nach dem Vielfachen des Argumentes. *Arch. Math. Phys.* **23**, 193–219. (Tragically von Ignatovsky was repressed by the Stalin regime in 1942.)
12. von Ignatovsky W. 1914 Zur theorie der gitter. *Ann. Phys.* **349**, 369–436. (doi:10.1002/andp.19143491103)
13. Twersky V. 1961 Elementary function representation of Schlömilch series. *Arch. Rat. Mech. Anal.* **8**, 323–332. (doi:10.1007/BF00277447)
14. Nörlund NE. 1924 *Vorlesungen über differenzenrechnung*, p. 53. Berlin, Germany: Springer.
15. Gradshtein IS, Ryzhik IM. 1980 *Table of integrals, series, and products*. New York, NY: Academic Press.
16. Abramovitz M, Stegun IA. 1965 *Handbook of mathematical functions*. New York, NY: Dower.
17. Abrahams E. 2010 *50 years of Anderson localization*. Singapore: World Scientific.
18. Sheng P. 2007 *Introduction to wave scattering, localization, and mesoscopic phenomena*. San Diego, CA: Academic.
19. Asatryan AA, Botten LC, Byrne MA, McPhedran RC, de Sterke CM. 2007 Evidence for a mobility edge for photons in two dimensions. *Phys. Rev. E* **75**, 015601. (doi:10.1103/PhysRevE.75.015601)
20. Anderson PW. 1972 More is different. *Science* **177**, 393–396. (doi:10.1126/science.177.4047.393)
21. Coates CV. 1885 Bessel's functions of the second order. *Q. J. Pure Appl. Math.* **20**, 250–260.
22. Wait JR. 1954 Reflection from a wire grid parallel to a conducting plane. *Can. J. Phys.* **32**, 571–579. (doi:10.1139/p54-061)
23. Lampe R, Klock P, Mayers P. 1985 Integral transforms useful for the accelerated summation of periodic, free-space Green's function. *IEEE Trans. Microwave Theory Tech.* **33**, 734–736. (doi:10.1109/TMTT.1985.1133067)
24. Achenbach JD, Li ZL. 1986 Reflection and transmission of scalar waves by a periodic array of screens. *Wave Motion* **8**, 225–234. (doi:10.1016/S0165-2125(86)80045-2)
25. Petit R. 1980 *Electromagnetic theory of gratings*. Berlin, Germany: Springer.
26. Jorgeson RE, Mittra R. 1990 Efficient calculation of the free space periodic Green's function. *IEEE Trans. Antennas Propagat.* **38**, 633–642. (doi:10.1109/8.53491)

27. Nicorovici NA, McPhedran RC, Petit R. 1994 Efficient calculation of the Green's function for electromagnetic scattering by gratings. *Phys. Rev. E* **49**, 4563–4577. (doi:10.1103/PhysRevE.49.4563)
28. Linton CM. 1998 The Green's function for two-dimensional Helmholtz equation in periodic domains. *J. Eng. Math.* **33**, 377–402. (doi:10.1023/A:1004377501747)
29. Erdelyi A. 1953 *Higher transcedental functions*, vol. 1, p. 30. New York, NY: McGraw-Hill.
30. Prudnikov AP, Brychkov YuA, Marychev OI. 1989 *More special functions*, vol. 3. New York, NY: Gordon and Breach.
31. Lewin L. 1981 *Polylogarithms and associated functions*. New York, NY: Elsevier Science.
32. Wolfram Research, Inc. 2014 *Mathematica, Version 10.0*. Champaign, IL: Wolfram Research, Inc.