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Schlömilch series and grating sums

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Abstract
We consider sums over the set of positive integers relevant to construction of periodic Green's functions for diffraction gratings and similar problems, and provide a general formula for a combination of Bessel functions of complex order and complex powers of distance from the origin. This general formula is investigated in a number of particular cases, and in particular we provide expressions which enable sums of functions with Neumann series to be re-expressed as combinations of hypergeometric series. We also investigate sums of Neumann functions of integer order, using analytic continuation techniques to provide formulae for their evaluation which we demonstrate are accurate and efficient in both the high and low frequency regions. We also exhibit sums which may be evaluated analytically, and recurrence formulae linking sums.

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1. Introduction

We consider here the use of the Poisson summation formula combined with an analytic continuation to give accurate and numerically efficient expressions for a wide class of sums over summands which combine Bessel functions, logarithms and powers of a positive integer. These sums arise in expressions for Green's functions for electrostatics, elastostatics, electromagnetism and elastodynamics [1], in the case where there is an infinite set of cylinders arranged periodically along a line to form a grating. Their accurate evaluation is required to permit multipole methods to be used to find transport properties and evaluate scattering properties of such gratings [1, 2].

There are extensive tabulations of sums of series of functions which contain Bessel functions, powers and other elementary functions [3], but there are gaps which relate to problems of physical importance. For example, there are well-established results for sums over the positive integers of Bessel functions J_m of argument an integer times a real scale factor and integral order m, but there are no formulae of equal simplicity for the corresponding sums of Neumann functions Y_m. However, both types of sums are found in cylindrical-harmonic expansions of Green's functions for the Helmholtz equation. Consequently, a number of authors have presented different techniques for evaluating these sums, with varying degrees of computational efficiency, algebraic complexity and region of applicability [4, 5]. In a recent work [6], we have shown how the use of the Poisson summation formula enables a Schlömilch series over the square array to be re-expressed as a hypergeometric series, and how this leads to a general method for evaluating double sums combining Bessel functions J_m, Y_m, powers of distance and possibly logarithms of distance, with in some cases closed form expressions being derived. Here we will perform a similar analysis for the case of one-dimensional sums, which have in some ways generated more algebraically-difficult summation formulae than the double sums, as the cited references indicate. We stress that the sums we deal with are often slowly or conditionally convergent, so that direct summation of them is generally impracticable, except as a means of verifying general formulae in particular cases. The basic technique for dealing with this is an analytic continuation, which we will see to be effective in a wide range of cases.

We commence by studying a Schlömilch series of general form over the positive integers, which we treat using the Poisson summation formula, and express as a series of hypergeometric type, in which the sums over the positive integers have been evaluated analytically. We illustrate particular cases where the Schlömilch series can be summed analytically, as well as giving integral and differential recurrence relations for them.

We next consider single sums over Neumann functions, Y_m, where a partial derivative of the Schlömilch series is required. We obtain highly accurate and efficient expressions for the sums of Y_0 and more generally Y_{2m} for m integral over the positive integers. The initial expressions we derive are useful only for low frequencies. However, we show that they may be analytically continued into the high-frequency region, and we demonstrate that the resulting expressions can be accurately and quickly evaluated even for normalized frequencies of several thousand. We comment also on the connection between sums of J_m and Y_m functions, where the relationship differs in an interesting fashion for single and double sums. In the appendix, we discuss briefly the connection between these grating sums and the density of states function.

2. Analytic expressions for a general class of grating sums

We consider a sum over the positive integers h of quite general form combining the Bessel function J and a power of h:

$$\mathcal{G}_{\lambda,\nu}(\xi) = \sum_{h=1}^{\infty} \frac{J_\lambda(2\pi h\xi)}{(2\pi h)^\nu}, \tag{1}$$

where the indices λ and μ are integer, real or complex numbers. The parameter ξ is taken to be real and positive. We assume initially that $\mathrm{Re}(\lambda) > \mathrm{Re}(\nu)$, so that $h = 0$ can be included in $\mathcal{G}$ without changing its value (although this assumption will be dispensed with later) and we may write (1) in the form

$$\mathcal{G}_{\lambda,\nu}(\xi) = \frac{1}{2} \sum_{h=-\infty}^{\infty} \frac{J_\lambda(2\pi|h|\xi)}{(2\pi|h|)^\nu}. \tag{2}$$

From the Poisson summation formula,

$$\mathcal{G}_{\lambda,\nu}(\xi) = \frac{1}{2\pi} \sum_p \int_0^\infty \frac{J_\lambda(\kappa\xi)}{\kappa^\nu} \cos(p\kappa)\, \mathrm{d}\kappa. \tag{3}$$

We evaluate the integral for $p \neq 0$ using a result from Prudnikov *et al* [3]:

$$\int_0^\infty \frac{J_\lambda(ax)\cos(bx)}{x^\nu}\,\mathrm{d}x = -\frac{\Gamma(1+\lambda-\nu)}{\Gamma(1+\lambda)}\left(\frac{a}{2}\right)^\lambda |b|^{-1-\lambda+\nu}\sin\left[\frac{\pi}{2}(\lambda-\nu)\right] \tag{4}$$

$$\times\,{}_2F_1\left[\frac{1}{2}(1+\lambda-\nu),\frac{1}{2}(2+\lambda-\nu);1+\lambda;\frac{a^2}{b^2}\right] \tag{5}$$

valid provided that $a \geqslant 0$, $a^2/b^2 < 1$, $\mathrm{Re}(\nu) < 1+\mathrm{Re}(\lambda)$. The integral we require for $p = 0$ is

$$\int_0^\infty \frac{J_\lambda(\kappa\xi)}{\kappa^\nu}\,\mathrm{d}\kappa = \frac{\xi^{\nu-1}}{2^\nu}\frac{\Gamma((\lambda-\nu+1)/2)}{\Gamma((\lambda+\nu+1)/2)}, \tag{6}$$

valid for $\mathrm{Re}(\nu) > -1/2$, $\xi \geqslant 0$, $\mathrm{Re}(\nu) < 1+\mathrm{Re}(\lambda)$. Consequently,

$$\begin{aligned}\mathcal{G}_{\lambda,\nu}(\xi) = \frac{1}{4\pi}\Bigg\{&\left(\frac{\xi}{2}\right)^{\nu-1}\frac{\Gamma((\lambda-\nu+1)/2)}{\Gamma((\lambda+\nu+1)/2)} - 4\frac{\Gamma(1+\lambda-\nu)}{\Gamma(1+\lambda)}\left(\frac{\xi}{2}\right)^\lambda\\ &\times\sum_{p=1}^\infty \frac{1}{p^{1+\lambda-\nu}}\sin\left[\frac{\pi}{2}(\lambda-\nu)\right]{}_2F_1\left[\frac{1}{2}(1+\lambda-\nu),\frac{1}{2}(2+\lambda-\nu);1+\lambda;\frac{\xi^2}{p^2}\right]\Bigg\}.\end{aligned} \tag{7}$$

We complete this derivation using the series expansion for the hypergeometric function, and replacing the sums over inverse powers of p by the appropriate Riemann zeta function. The result is

$$\begin{aligned}\mathcal{G}_{\lambda,\nu}(\xi) = {}&\frac{1}{4\pi}\left(\frac{\xi}{2}\right)^{\nu-1}\frac{\Gamma((\lambda-\nu+1)/2)}{\Gamma((\lambda+\nu+1)/2)}\\ &-\frac{1}{\pi}\frac{\Gamma(1+\lambda-\nu)}{\Gamma((1+\lambda-\nu)/2)\Gamma((2+\lambda-\nu)/2)}\left(\frac{\xi}{2}\right)^\lambda\sin\left[\frac{\pi}{2}(\lambda-\nu)\right]\\ &\times\sum_{n=0}^\infty\frac{\Gamma((\lambda-\nu+1+2n)/2)\Gamma((\lambda-\nu+2+2n)/2))}{\Gamma(1+\lambda+n)\Gamma(1+n)}\zeta(2n+1+\lambda-\nu)\xi^{2n}.\end{aligned} \tag{8}$$

Note that the hypergeometric series on the right-hand side of (8) converges absolutely provided that $\xi < 1$, and thus by an analytic continuation provides a meaning to the left-hand side for all complex values of λ and ν. Expression (8) may be simplified by two applications of the duplication formula for the Gamma function:

$$\begin{aligned}\mathcal{G}_{\lambda,\nu}(\xi) = {}&\frac{1}{4\pi}\left(\frac{\xi}{2}\right)^{\nu-1}\frac{\Gamma((\lambda-\nu+1)/2)}{\Gamma((\lambda+\nu+1)/2)} - \frac{1}{\pi}\left(\frac{\xi}{2}\right)^\lambda\sin\left[\frac{\pi}{2}(\lambda-\nu)\right]\\ &\times\sum_{n=0}^\infty\frac{\Gamma(2n+1+\lambda-\nu)}{\Gamma(1+\lambda+n)\Gamma(1+n)}\zeta(2n+1+\lambda-\nu)\left(\frac{\xi}{2}\right)^{2n}.\end{aligned} \tag{9}$$

Expression (9) has a number of important features. It is very general, in that λ and ν are the arbitrary complex parameters, and as we will see can give analytic results for certain grating sums in special cases, and can be used to derive recurrence relations among sums. Differentiation of (9) with respect to the parameters can yield expressions for related grating sums, as we will illustrate in section 3. Its main drawback is its limitation that the frequency parameter ξ be less than unity, but we will show in section 4 how this can be overcome by Kummer's method of adding and subtracting a sum whose result is known analytically.

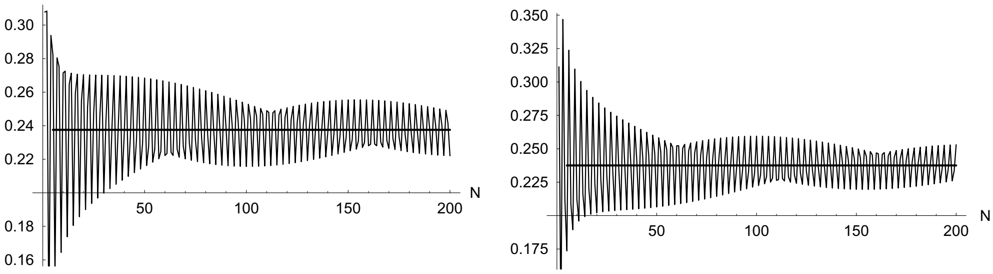

Figure 1. Comparison of the partial sums over N terms ($N \in [1, 200]$) for the left-hand sides of (15) for $l = 1$ (left) and $l = 2$ (right) and the right-hand sides (solid horizontal line), at $\xi = 0.67$.

As our first special case of (9), we take the limit as $\lambda \to \nu$. Then the sine factor multiplying the series ensures all terms apart from $n = 0$ do not contribute to the limit. For that term, we use the expansion of ζ near its singularity when its argument is unity:

$$\zeta(1 + \lambda - \nu) \simeq \frac{1}{\lambda - \nu} + \gamma + \cdots, \qquad \text{for} \quad \lambda \to \nu. \tag{10}$$

The result is

$$\mathcal{G}_{\nu,\nu}(\xi) = \frac{1}{4\sqrt{\pi}\Gamma(\nu + 1/2)} \left(\frac{\xi}{2}\right)^{\nu-1} - \frac{1}{2\Gamma(1 + \nu)} \left(\frac{\xi}{2}\right)^{\nu}. \tag{11}$$

An important particular case of (11) is for $\nu = 0$:

$$\mathcal{G}_{0,0}(\xi) = \sum_{h=1}^{\infty} J_0(2\pi\xi h) = \frac{1}{2\pi\xi} - \frac{1}{2}. \tag{12}$$

An even simpler case arises for $\lambda = \nu + 2l$, where l is a positive integer. Then the sine term ensures all terms in the series in (9) make zero contribution, so that

$$\mathcal{G}_{\nu+2l,\nu}(\xi) = \frac{1}{4\pi} \left(\frac{\xi}{2}\right)^{\nu-1} \frac{\Gamma(l + 1/2)}{\Gamma(\nu + l + 1/2)}. \tag{13}$$

We next put $\nu = 0$, to obtain

$$\mathcal{G}_{\lambda,0}(\xi) = \frac{1}{2\pi\xi} - \frac{1}{\pi} \left(\frac{\xi}{2}\right)^{\lambda} \sin\left(\frac{\pi\lambda}{2}\right) \sum_{n=0}^{\infty} \frac{\Gamma(2n + 1 + \lambda)}{\Gamma(1 + \lambda + n)\Gamma(1 + n)} \zeta(2n + 1 + \lambda) \left(\frac{\xi}{2}\right)^{2n}. \tag{14}$$

For $\lambda = 0$, this agrees with (12). For $\lambda = 2l$, with l as a positive integer, the series does not contribute, so that we find

$$\mathcal{G}_{2l,0}(\xi) = \sum_{h=1}^{\infty} J_{2l}(2\pi\xi h) = \frac{1}{2\pi\xi}. \tag{15}$$

We present numerical confirmation of (15) in figure 1. For direct summation up to $h = 200$, the mean of the results for $l = 1$ and $l = 2$ are respectively 0.237 888 and 0.237 702, in good accord with the analytic value 0.237 545. Note that Prudnikov *et al* [3] give the following result:

$$\sum_{h=1}^{\infty} J_{2n}(hx) = \frac{1}{x} - \frac{1}{2} + 2\sum_{l=1}^{m} \frac{1}{\sqrt{x^2 - 4l^2\pi^2}} \cos\left(2n \arcsin\frac{2l\pi}{x}\right), \tag{16}$$

where $2m\pi < x < 2(m+1)\pi$. In (15) we have assumed $\xi < 1$, so that (16) and (15) are in accord, except that there is evidently a Kronecker delta $\delta_{n,0}$ omitted from the factor of $(1/2)$ in (16). We comment further on the term represented by the the sum over h in (16) in section 4.

The form of (14) for $\lambda = 2l+1$, $l \geqslant 0$, is

$$\mathcal{G}_{2l+1,0}(\xi) = \frac{1}{2\pi\xi} - \frac{(-1)^l}{\pi}\left(\frac{\xi}{2}\right)^{2l+1}\sum_{n=0}^{\infty}\frac{\Gamma(2n+2l+2)}{\Gamma(2l+n+2)\Gamma(1+n)}\zeta(2n+2l+2)\left(\frac{\xi}{2}\right)^{2n}. \quad (17)$$

The grating sums $\mathcal{G}$ obey four recurrence relations, similar to those for double sums [7]:

$$\mathcal{G}_{\lambda+1,\nu+1}(\xi) = \frac{1}{\xi^{\lambda+1}}\int_0^{\xi}\eta^{\lambda+1}\mathcal{G}_{\lambda,\nu}(\eta)\,\mathrm{d}\eta \quad (18)$$

valid for $\mathrm{Re}(\lambda) > -1/2$ and $\mathrm{Re}(\lambda+\nu) > -1$, and

$$\mathcal{G}_{\lambda-1,\nu+1}(\xi) = \frac{1}{\pi}\left(\frac{\xi}{2}\right)^{\lambda-1}\sin\left[(\lambda-\nu)\frac{\pi}{2}\right]\frac{\Gamma(\lambda-\nu-1)}{\Gamma(\lambda)}\zeta(\lambda-\nu-1) - \xi^{\lambda-1}\int_0^{\xi}\frac{\mathcal{G}_{\lambda,\nu}(\eta)}{\eta^{\lambda-1}}\,\mathrm{d}\eta, \quad (19)$$

valid for $\mathrm{Re}(\nu-\lambda+1) > 0$. These act by integration, and increase the second subscript. The two differential relations are

$$\mathcal{G}_{\lambda-1,\nu-1}(\xi) = \xi^{-\lambda}[\xi^{\lambda}\mathcal{G}_{\lambda,\nu}(\xi)]', \quad (20)$$

and

$$\mathcal{G}_{\lambda+1,\nu-1}(\xi) = -\xi^{\lambda}[\xi^{-\lambda}\mathcal{G}_{\lambda,\nu}(\xi)]', \quad (21)$$

both of which decrease the second subscript. Appropriate pairwise combinations of these act on either the first or the second subscript alone:

$$\mathcal{G}_{\lambda+2,\nu}(\xi) = \frac{2(\lambda+1)}{\xi^{\lambda+2}}\int_0^{\xi}\eta^{\lambda+1}\mathcal{G}_{\lambda,\nu}(\eta)\,\mathrm{d}\eta - \mathcal{G}_{\lambda,\nu}(\xi), \quad (22)$$

$$\begin{aligned}\mathcal{G}_{\lambda,\nu}(\xi) = {} & -\frac{1}{\pi}\left(\frac{\xi}{2}\right)^{\lambda}\sin\left[\frac{\pi}{2}(\lambda-\nu)\right]\frac{\Gamma(\lambda-\nu+1)}{\Gamma(\lambda+1)}\zeta(\lambda-\nu+1)\\ & - 2(\lambda+1)\xi^{\lambda}\int_0^{\xi}\frac{\mathcal{G}_{\lambda+2,\nu}(\eta)}{\eta^{\lambda+1}}\,\mathrm{d}\eta - \mathcal{G}_{\lambda+2,\nu}(\xi),\end{aligned} \quad (23)$$

which are the inverse operations on the first subscript. The lowering and raising relations for the second subscript are

$$\mathcal{G}_{\lambda,\nu-2}(\xi) = \frac{\lambda^2}{\xi^2}\mathcal{G}_{\lambda,\nu}(\xi) - \frac{1}{\xi}\mathcal{G}'_{\lambda,\nu}(\xi) - \mathcal{G}''_{\lambda,\nu}(\xi) \quad (24)$$

and

$$\begin{aligned}\mathcal{G}_{\lambda,\nu+2}(\xi) = {} & \frac{1}{\pi}\left(\frac{\xi}{2}\right)^{\lambda}\sin\left[\frac{\pi}{2}(\lambda-\nu)\right]\frac{\Gamma(\lambda-\nu-1)}{\Gamma(\lambda+1)}\zeta(\lambda-\nu-1)\\ & - \xi^{\lambda}\int_0^{\xi}\frac{\mathrm{d}\eta}{\eta^{2\lambda+1}}\int_0^{\eta}\mathrm{d}\tau\,\tau^{\lambda+1}\mathcal{G}_{\lambda,\nu}(\tau).\end{aligned} \quad (25)$$

We can verify that expression (9) satisfies each of the recurrence relations (18)–(21). The algebra is elementary, with the exception of (19), where an additional term needs to be added to the hypergeometric series to fill in for the lowest order term (all other terms having been increased in order by integration). We can thus use either the recurrence relations or the hypergeometric expression (9) in order to extend the calculation of the $\mathcal{G}_{\lambda,\nu}(\xi)$ from the region of derivation over the whole range of the two complex variables λ and ν. Note the structure of (9); the first term will have simple poles at $\lambda - \nu + 1 = -2m$, where m is a positive integer. In the series over n in the second term, poles of $\Gamma(2n+1+\lambda-\nu)$ for the argument a negative integer are counterbalanced by zeros of $\sin[\pi(\lambda-\nu)/2]$ or $\zeta(2n+1+\lambda-\nu)$. A pole will occur only for $n = m$, where $\lambda - \nu + 1 = -2m$, and this pole exactly cancels out the pole in the first term.

As an example of the use of the recurrence relations, we have from (11) that

$$\mathcal{G}_{1,1}(\xi) = \frac{1}{2\pi} - \frac{\xi}{4}, \tag{26}$$

and this gives in (19)

$$\mathcal{G}_{0,2}(\xi) = \frac{\xi^2}{8} - \frac{\xi}{2\pi} + \frac{1}{24}. \tag{27}$$

We can get the same result from (12) and (25).

Another result we will need below comes from (9), combining the first term on the right-hand side with the $n = 0$ term in the sum, as described above:

$$\mathcal{G}_{0,1}(\xi) = -\frac{1}{2\pi}\log(\pi\xi) + \frac{1}{\pi}\sum_{n=1}^{\infty}\frac{\Gamma(2n)}{[\Gamma(1+n)]^2}\zeta(2n)\left(\frac{\xi}{2}\right)^n. \tag{28}$$

3. Series combining Bessel functions and logarithms

From definition (1) we can construct related series by differentiation with respect to parameters. For example, by differentiation with respect to ν, we obtain a general formula for sums combining a logarithm with a Bessel function and a power of the distance:

$$\mathcal{L}_{\lambda,\nu}(\xi) = -\frac{\partial}{\partial\nu}\mathcal{G}_{\lambda,\nu}(\xi) = \sum_{h=1}^{\infty}\log(2\pi h)\frac{J_\lambda(2\pi h\xi)}{(2\pi h)^\nu}. \tag{29}$$

Using expansion (9), we find

$$\begin{aligned}\mathcal{L}_{\lambda,\nu}(\xi) = {} & -\frac{1}{4\pi}\frac{\Gamma((\lambda-\nu+1)/2)}{\Gamma((\lambda+\nu+1)/2)}\left[\log\left(\frac{\xi}{2}\right) - \frac{1}{2}\psi\left(\frac{\lambda-\nu+1}{2}\right) - \frac{1}{2}\psi\left(\frac{\lambda+\nu+1}{2}\right)\right] \\ & - \frac{1}{2}\left(\frac{\xi}{2}\right)^\lambda \cos\left[\frac{\pi(\lambda-\nu)}{2}\right]\sum_{n=0}^{\infty}\frac{\Gamma(2n+1+\lambda-\nu)\zeta(2n+1+\lambda-\nu)}{\Gamma(1+\lambda+n)\Gamma(1+n)}\left(\frac{\xi}{2}\right)^{2n} \\ & - \frac{1}{\pi}\left(\frac{\xi}{2}\right)^\lambda \sin\left[\frac{\pi(\lambda-\nu)}{2}\right]\sum_{n=0}^{\infty}\frac{\Gamma(2n+1+\lambda-\nu)}{\Gamma(1+\lambda+n)\Gamma(1+n)}\left(\frac{\xi}{2}\right)^{2n} \\ & \times[\psi(2n+1+\lambda-\nu)\zeta(2n+1+\lambda-\nu) + \zeta'(2n+1+\lambda-\nu)].\end{aligned} \tag{30}$$

This expression could be used, for example, with the Neumann series for the Bessel function $Y_\eta(2\pi h\xi)$ to generate expressions for sums containing $J_\lambda(2\pi h\xi)Y_\eta(2\pi h\xi)$, which could arise in nonlinear grating problems in photonics.

Let us evaluate $\mathcal{L}_{0,0}$:

$$\mathcal{L}_{0,0}(\xi) = -\frac{1}{2\pi\xi}\log\left(\frac{\xi}{2}\right) + \frac{\psi(1/2)}{2\pi\xi} - \frac{1}{2}\sum_{n=1}^{\infty}\frac{\Gamma(2n+1)}{\Gamma(1+n)^2}\zeta(2n+1)\left(\frac{\xi}{2}\right)^{2n}. \tag{31}$$

A numerical demonstration of this result is given in figure 2, where the mean of the sample obtained by summing over lines of length going up to 200 is −0.469 976, while (30) gives −0.469 045.

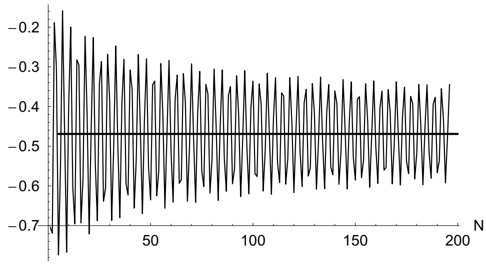

Figure 2. Partial sums over N terms ($N \in [1, 200]$) for $\mathcal{L}_{0,0}(\xi)$, at $\xi = 0.73$, with the analytical result (31) being indicated by the solid horizontal line.

4. Series of Neumann functions

These are needed to construct Green's functions for the Helmholtz equation [5–8]. We start with a convenient formula for the Neumann functions of integer order [9]

$$Y_n(z) = \frac{2}{\pi}\left[\frac{\partial J_\lambda(z)}{\partial\lambda}\right]_{\lambda=n} - \frac{n!}{\pi}\sum_{l=0}^{n-1}\frac{J_l(z)}{(n-l)l!}\left(\frac{2}{z}\right)^{n-l}. \tag{32}$$

Defining

$$\mathcal{Y}_{n,\nu}(\xi) = \sum_{h=1}^{\infty}\frac{Y_n(2\pi h\xi)}{(2\pi h)^\nu}, \tag{33}$$

we find from (1) and (32) that

$$\mathcal{Y}_{n,\nu}(\xi) = \frac{2}{\pi}\left[\frac{\partial \mathcal{G}_{\lambda,\nu}(\xi)}{\partial\lambda}\right]_{\lambda=n} - \frac{n!}{\pi}\sum_{l=0}^{n-1}\frac{\mathcal{G}_{l,n-l+\nu}}{(n-l)l!}\left(\frac{2}{\xi}\right)^{n-l}. \tag{34}$$

We will consider hereafter the case $\nu = 0$. From (14), we find

$$\begin{aligned}\frac{2}{\pi}\left[\frac{\partial \mathcal{G}_{\lambda,0}(\xi)}{\partial\lambda}\right]_{\lambda=n} &= -\frac{1}{\pi}\cos\left(\frac{\pi n}{2}\right)\sum_{m=0}^{\infty}\frac{\Gamma(2m+1+n)}{\Gamma(1+m+n)\Gamma(1+m)}\zeta(2m+1+n)\left(\frac{\xi}{2}\right)^{2m+n}\\ &\quad - \frac{2}{\pi^2}\sin\left(\frac{\pi n}{2}\right)\sum_{m=0}^{\infty}\frac{\Gamma(2m+1+n)}{\Gamma(1+m+n)\Gamma(1+m)}\left(\frac{\xi}{2}\right)^{2m+n} g(n,m,\xi),\end{aligned} \tag{35}$$

where

$$g(n,m,\xi) = \left[\log\left(\frac{\xi}{2}\right) + \psi(2m+1+n) - \psi(m+1+n)\right]\zeta(2m+1+n) + \zeta'(2m+1+n).$$

From (35), expression (34) gives simpler results for n even than for n odd, and we note that only the former arise in scattering problems involving a plane wave incident normally on a grating. We start with $n = 0$, for which only the partial derivative in (34) contributes. The terms in (35) for $m = 0$ have to be dealt with using (10); first we have to set $m = 0$ and then take the limit $n \to 0$. The result is

$$\mathcal{Y}_{0,0}(\xi) = \sum_{h=1}^{\infty} Y_0(2\pi h\xi) = -\frac{1}{\pi}\left[\log\left(\frac{\xi}{2}\right) + \gamma\right] - \frac{1}{\pi}\sum_{m=1}^{\infty}\frac{\Gamma(2m+1)}{[\Gamma(1+m)]^2}\zeta(2m+1)\left(\frac{\xi}{2}\right)^{2m}. \tag{36}$$

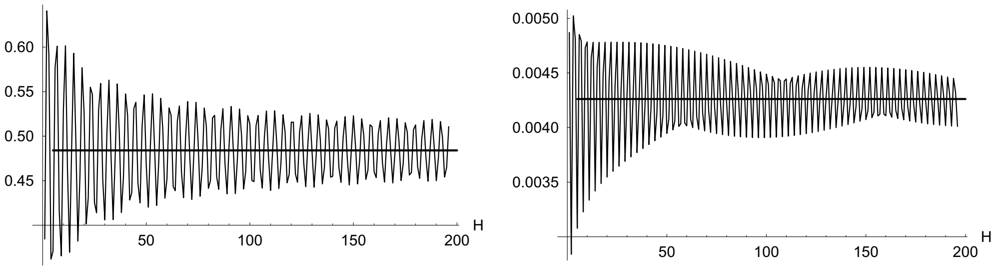

Figure 3. Partial sums over H terms ($H \in [1, 200]$) for $\mathcal{Y}_{0,0}(\xi)$, at $\xi = 0.237$ (left), with the analytic result (36) being given by the horizontal line, and at $\xi = 2555.33$ (right), with the analytic result (43) for $N = 3200$ being given by the horizontal line.

As a numerical example, we show in figure 3 (left) the partial sums over H terms for $\mathcal{Y}_{0,0}(\xi)$, with H up to 200. The analytic result (36) gives with $\xi = 0.237$ the value 0.484 02; the mean of the values from partial sums is 0.484 23.

Note that the series in (36) has a radius of convergence of unity, which restricts its utility. To extend the radius of convergence we write (36) in a different form. First we observe that by replacing ξ by a complex argument $z \in \mathbb{C}$ the series in (36) is absolutely convergent inside the domain $D_1 = \{z : 0 < |z| < 1\}$. Then, we substitute the ζ function from (36) by its definition series, change the order of summation, and apply the Binomial theorem

$$\frac{1}{\sqrt{1-(z/n)^2}} = \sum_{m=0}^{\infty} \frac{\Gamma(2m+1)}{[\Gamma(m+1)]^2}\left(\frac{z}{2n}\right)^{2m}, \tag{37}$$

which is valid for $|z| < n$. Thus, for the case $|z| < 1$, we may rewrite (36) in the form

$$\widetilde{\mathcal{Y}}_{0,0}(z) = -\frac{1}{\pi}\left[\log\left(\frac{z}{2}\right)+\gamma\right] - \frac{1}{\pi}\sum_{n=1}^{\infty}\left[\frac{1}{\sqrt{n^2-z^2}} - \frac{1}{n}\right]. \tag{38}$$

The complex function $\widetilde{\mathcal{Y}}_{0,0}(z)$ is defined everywhere in the complex plane except the points $z = 0, \pm 1, \ldots, \pm n, \ldots,$ located on the real axis, and represents the analytic continuation of (36) in $\mathbb{C}$.

For real z ($z = \xi, 0 < \xi < 1$), equation (38) is identical with (31) in [10] if we consider $S_0^Y(k, d)/2$, with $k = 2\pi\xi < 2\pi$, $K = 2\pi$, $d = 1$, $\alpha_n = 2\pi n$ and $|\chi_n|^2 = \alpha_n^2 - k^2$. In [10] we showed that for an arbitrarily large value of ξ we may use the formula

$$\begin{aligned}
\frac{1}{2}S_0^Y(\xi) &= \sum_{h=1}^{\infty} Y_0(2\pi h\xi) \\
&= -\frac{1}{\pi}\left[\log\left(\frac{\xi}{2}\right)+\gamma\right] - \frac{1}{\pi}\left\{\sum_{n=N+1}^{\infty}\left[\frac{1}{\sqrt{n^2-\xi^2}} - \frac{1}{n}\right] - \sum_{n=1}^{N}\frac{1}{n}\right\} \\
&= -\frac{1}{\pi}\left[\log\left(\frac{\xi}{2}\right) - \psi(N+1)\right] - \frac{1}{\pi}\sum_{n=N+1}^{\infty}\left[\frac{1}{\sqrt{n^2-\xi^2}} - \frac{1}{n}\right],
\end{aligned} \tag{39}$$

where $0 < N < \xi < N+1$, with N integer. We now extend the radius of convergence of (36) to $\xi = N+1$, by considering the analytic continuation (38) in the form

$$\widetilde{\mathcal{Y}}_{0,0}(z) = -\frac{1}{\pi}\left[\log\left(\frac{z}{2}\right) - \psi(N+1) + \sum_{n=1}^{N}\frac{1}{\sqrt{n^2-z^2}}\right] - \frac{1}{\pi}\sum_{n=N+1}^{\infty}\left[\frac{1}{\sqrt{n^2-z^2}} - \frac{1}{n}\right], \tag{40}$$

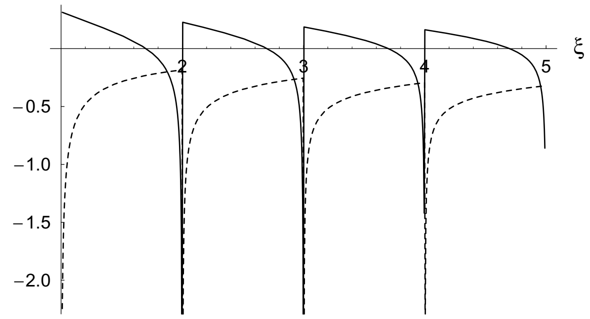

Figure 4. The real (solid line) and imaginary (dashed line) parts of $\widetilde{\mathcal{Y}}_{0,0}(\xi)$ obtained from the analytic result (43), for ξ in the range of 1–5.

with $z = \xi$ (real). A direct comparison of (40) and (39) shows that

$$\tfrac{1}{2}S_0^Y(\xi) = \mathrm{Re}[\widetilde{\mathcal{Y}}_{0,0}(\xi)], \qquad \xi \in (0, N+1)\backslash\{1, 2, \ldots, N\}. \tag{41}$$

Now, for $n \geqslant N+1$ we may use the Binomial theorem (37) to write the series in (40) in a form similar to that in (36). Let us denote

$$\zeta_N^\infty(n) = \sum_{l=N+1}^{\infty} \frac{1}{l^n} = \frac{(-1)^n \psi^{(n-1)}(N+1)}{(n-1)!}, \tag{42}$$

using the definition of polygamma function [9]. Then, we may show that

$$\widetilde{\mathcal{Y}}_{0,0}(\xi) = -\frac{1}{\pi}\left[\log\left(\frac{\xi}{2}\right) - \psi(N+1) + \sum_{l=1}^{N} \frac{1}{\sqrt{l^2-\xi^2}}\right] - \frac{1}{\pi}\sum_{n=1}^{\infty} \frac{\Gamma(2n+1)}{[\Gamma(n+1)]^2}\zeta_N^\infty(2n+1)\left(\frac{\xi}{2}\right)^{2n}, \tag{43}$$

the radius of convergence of (43) being $\xi = N+1$, dictated by the first term in (42).

The terms in the series in (39) converge as $1/n^2$ while the series in (43) converges as $\mathrm{e}^{-2n\log(N/\xi)}/n^{3/2}$ (this expression has been derived by using Stirling's formula for the Gamma functions in (43), and approximating ζ_N^∞ by an integral). Accordingly, expression (43) works very well, as we show in an example in figure 3 (right) for $\xi = 2555.33$, where once again the partial sums and the analytic result agree well (the mean of the partial sum values shown is 0.004 2609, while (43) gives 0.004 2614). The value of N used in figure 3 (right) was 3200, and should be chosen to significantly exceed ξ to guarantee good convergence of the sum over n in (43) (although of course the converged result is independent of the choice of N as long as $N > \xi$). Also, we need only 100 terms for the series in (43) while, using the corresponding accelerated series given in [10] for (39), we have to sum 200 000 terms to obtain good convergence of the numerical result, accurate to eight significant figures. For $\xi = 55.33$ we obtained an accuracy of ten significant figures using $N = 150$ and 20 terms for the series in (43), while the same result was obtained from (39) summing 50 000 terms.

Note that result (43) has a nonzero imaginary part for $\xi > 1$. This is shown in figure 4, where the real and imaginary parts of $\widetilde{\mathcal{Y}}_{0,0}(\xi)$ are shown for ξ ranging from one to five. From (43), and choosing the sign of the imaginary square root in accordance with the data of figure 4, we see that

$$\mathrm{Im}[\widetilde{\mathcal{Y}}_{0,0}(\xi)] = \frac{1}{\pi}\sum_{l=1}^{\lfloor\xi\rfloor} \frac{1}{\sqrt{\xi^2-l^2}}. \tag{44}$$

Comparing (44) and (16), we obtain

$$\frac{1}{2}S_0^J(\xi) = \sum_{h=1}^{\infty} J_0(2\pi h\xi) = \frac{1}{2\pi\xi} - \frac{1}{2} + \mathrm{Im}[\widetilde{\mathcal{Y}}_{0,0}(\xi)], \qquad \xi \in (0, N+1)\backslash\{1, 2, \ldots, N\}. \tag{45}$$

Expressions (44) and (45) arise in connection with density of states functions and are discussed further in the appendix.

One aspect of (44) which deserves comment is that (33) defines a real-valued function, while (43) is a complex function if $\xi > 1$. The imaginary part for $\widetilde{\mathcal{Y}}_{0,0}(\xi)$ has been acquired in the process of the analytic continuation of a definition valid only for $\xi < 1$ into the region $\xi > 1$.

It is interesting to compare the one-dimensional sum (45) with the corresponding results in two dimensions [11] and three dimensions [12]:

$$\sum_{h_1,h_2}{}' J_0\big(2\pi\xi\sqrt{h_1^2+h_2^2}\big) = -1, \tag{46}$$

$$\sum_{h_1,h_2,h_3}{}' J_0\big(2\pi\xi\sqrt{h_1^2+h_2^2+h_3^2}\big) = -1/\sqrt{4\pi}, \tag{47}$$

where the prime means that the origin is excluded from the sum. The right-hand sides in two and three dimensions are not ξ dependent, since no square root factors occur in the lattice sums to cross-couple J and Y series.

Let us now evaluate

$$\mathcal{Y}_{1,0}(\xi) = \frac{2}{\pi}\left[\frac{\partial \mathcal{G}_{\lambda,0}(\xi)}{\partial\lambda}\right]_{\lambda=1} - \frac{2}{\pi\xi}\mathcal{G}_{0,1}(\xi). \tag{48}$$

Using (35) and (28), we obtain

$$\mathcal{Y}_{1,0}(\xi) = -\frac{1}{\pi^2\xi}\log(\pi\xi) - \frac{2}{\pi^2}\sum_{m=0}^{\infty}\frac{\Gamma(2m+2)}{\Gamma(2+m)\Gamma(1+m)}\left(\frac{\xi}{2}\right)^{2m+1}$$
$$\times\left\{\left[\log\left(\frac{\xi}{2}\right) + \psi(2m+3) - \psi(m+2)\right]\zeta(2m+2) + \zeta'(2m+2)\right\}. \tag{49}$$

If we consider the case $n = 2$ in (34), we find using (26) and (27) that

$$\mathcal{Y}_{2,0}(\xi) = \frac{1}{\pi}\sum_{m=0}^{\infty}\frac{\Gamma(2m+3)}{\Gamma(m+3)\Gamma(m+1)}\zeta(2m+3)\left(\frac{\xi}{2}\right)^{2m+2} - \frac{4}{\pi\xi^2}\mathcal{G}_{0,2}(\xi) - \frac{4}{\pi\xi}\mathcal{G}_{1,1}(\xi), \tag{50}$$

or

$$\mathcal{Y}_{2,0}(\xi) = -\frac{1}{6\pi\xi^2} + \frac{1}{2\pi} + \frac{1}{\pi}\sum_{m=1}^{\infty}\frac{\Gamma(2m+1)}{\Gamma(m+2)\Gamma(m)}\zeta(2m+1)\left(\frac{\xi}{2}\right)^{2m}. \tag{51}$$

The same expression can be derived from the recurrence relation

$$\mathcal{Y}_{\lambda+2,\nu}(\xi) = \frac{(2\lambda+2)}{\xi^{\lambda+2}}\int_0^{\xi}\eta^{\lambda+1}\mathcal{Y}_{\lambda,\nu}(\eta)\,\mathrm{d}\eta - \mathcal{Y}_{\lambda,\nu}(\xi) - \frac{\Gamma(\lambda+2)\zeta(\lambda+\nu+2)}{\pi^{\lambda+\nu+3}2^{\nu}\xi^{\lambda+2}}, \tag{52}$$

applied to (36).

One advantage of the use of recurrence relations is that we can substitute into them the extended-convergence expression in place of the expression with unit radius of convergence. Thus, using (43) in (52), we find the analytic continuation of (51):

$$\widetilde{\mathcal{Y}}_{2,0}(\xi) = -\frac{1}{6\pi\xi^2} - \frac{N(N+1)}{\pi\xi^2} + \frac{1}{2\pi} + \frac{1}{\pi}\sum_{l=1}^{N}\frac{1}{\sqrt{l^2-\xi^2}}\left(\frac{2l^2}{\xi^2}-1\right) + \frac{1}{\pi}\sum_{m=1}^{\infty}\frac{\Gamma(2m+1)}{\Gamma(m+2)\Gamma(m)}\zeta_N^{\infty}(2m+1)\left(\frac{\xi}{2}\right)^{2m}. \tag{53}$$

The series in (53) converges as

$$\frac{1}{2\sqrt{\pi}\sqrt{m}(m+1)}\exp(-2(m+1)\log(N/\xi) - 3/(2m)) \propto \frac{1}{m^{3/2}}\exp(-2m\log(N/\xi)). \tag{54}$$

As a numerical example, with $\xi = 0.237$, direct summation up to 200 terms gives a mean of $-0.780\,113$, while (53) gives the value $-0.779\,698$, independent of N. Note also for the term in (53) which can become imaginary,

$$\frac{1}{\pi}\sum_{l=1}^{N}\frac{1}{\sqrt{l^2-\xi^2}}\left(\frac{2l^2}{\xi^2}-1\right) = -\frac{1}{\pi}\sum_{l=1}^{N}\frac{1}{\sqrt{l^2-\xi^2}}\cos\left[2\arcsin\left(\frac{l}{\xi}\right)\right], \tag{55}$$

leading to a result in keeping with (16)

$$\mathcal{G}_{2,0}(\xi) = \sum_{h=1}^{\infty} J_2(2\pi\xi h) = \frac{1}{2\pi\xi} + \mathrm{Im}[\widetilde{\mathcal{Y}}_{2,0}(\xi)]. \tag{56}$$

The result for $n = 4$ is

$$\mathcal{Y}_{4,0}(\xi) = -\frac{1}{15\pi\xi^4} - \frac{1}{3\pi\xi^2} + \frac{1}{4\pi} - \frac{1}{\pi}\sum_{m=2}^{\infty}\frac{\Gamma(2m+1)}{\Gamma(m+3)\Gamma(m-1)}\zeta(2m+1)\left(\frac{\xi}{2}\right)^{2m}. \tag{57}$$

To derive this from (34), we need the following sums:

$$\mathcal{G}_{3,1}(\xi) = \frac{1}{6\pi}, \qquad \mathcal{G}_{2,2}(\xi) = -\frac{\xi^2}{16} + \frac{\xi}{6\pi}, \qquad \mathcal{G}_{1,3}(\xi) = \frac{\xi^3}{32} - \frac{\xi^2}{6\pi} + \frac{\xi}{48},$$
$$\mathcal{G}_{0,4}(\xi) = -\frac{\xi^4}{128} + \frac{\xi^3}{18\pi} - \frac{\xi^2}{96} + \frac{1}{1440}. \tag{58}$$

The pattern of these results gives us the form of $\mathcal{Y}_{2n,0}(\xi)$:

$$\mathcal{Y}_{2n,0}(\xi) = -\frac{\Gamma(2n)\zeta(2n)}{\pi^{2n+1}\xi^{2n}} + \cdots + \frac{1}{2n\pi} + \frac{(-1)^{n+1}}{\pi}\sum_{m=n}^{\infty}\frac{\Gamma(2m+1)}{\Gamma(m+1+n)\Gamma(m+1-n)}\zeta(2m+1)\left(\frac{\xi}{2}\right)^{2m}. \tag{59}$$

Here the terms in inverse powers of ξ are of even order, and may be derived most easily using (52). Thus,

$$\mathcal{Y}_{2n,0}(\xi) = -\frac{|B_{2n}|2^{(2n-1)}}{2n\pi\xi^{2n}} + \cdots + \frac{1}{2n\pi} + \frac{(-1)^{n+1}\xi^{2n}}{2^{2n}\pi}\frac{\Gamma(2n+1)}{\Gamma(n+1/2)\Gamma(n+1)} \times \sum_{m=0}^{\infty}\frac{\Gamma(m+n+1/2)\Gamma(m+n+1)}{\Gamma(m+1+2n)\Gamma(m+1)}\zeta(2m+2n+1)\xi^{2m}, \tag{60}$$

where B_{2n} are the Bernoulli numbers. We can extend the radius of convergence of (60) using analytic continuation in the same way as (43) was derived. We thus deduce

$$\widetilde{\mathcal{Y}}_{2n,0}(\xi) = -\frac{|B_{2n}|2^{(2n-1)}}{2n\pi\xi^{2n}} + \cdots + \frac{1}{2n\pi} + \frac{(-1)^{n+1}}{\pi}\sum_{p=1}^{N}\frac{\xi^{2n}}{\sqrt{p^2-\xi^2}[p+\sqrt{p^2-\xi^2}]^{2n}}$$
$$+ \frac{(-1)^{n+1}\xi^{2n}}{2^{2n}\pi}\frac{\Gamma(2n+1)}{\Gamma(n+1/2)\Gamma(n+1)}\sum_{m=0}^{\infty}\frac{\Gamma(m+n+1/2)\Gamma(m+n+1)}{\Gamma(m+1+2n)\Gamma(m+1)}$$
$$\times \zeta_N^{\infty}(2m+2n+1)\xi^{2m}, \tag{61}$$

exploiting the result [9]

$$\frac{\Gamma(2n+1)}{\Gamma(n+1/2)\Gamma(n+1)}\sum_{m=0}^{\infty}\frac{\Gamma(m+n+1/2)\Gamma(m+n+1)}{\Gamma(m+1+2n)\Gamma(m+1)}\xi^{2m}$$
$$= F(n+1/2, n+1; 2n+1; \xi^2) = \frac{2^{2n}}{\sqrt{1-\xi^2}[1+\sqrt{1-\xi^2}]^{2n}}, \tag{62}$$

for n a positive integer. Equation (61) is the general extended-convergence expansion ($0 < \xi < N+1$) for $\mathcal{Y}_{2n,0}(\xi)$, obtained by analytic continuation of (60). Note that the series in (61) converges as

$$\frac{1}{2\sqrt{\pi}\sqrt{m}(m+n)}\exp(-2(m+n)\log(N/\xi) - n(2n+1)/(2m)) \propto \frac{1}{m^{3/2}}\exp(-2m\log(N/\xi)), \tag{63}$$

for $m \gg n$.

We can re-express the terms in the finite sum on the right-hand side of (61) as follows:

$$\frac{\xi^{2n}}{\sqrt{p^2-\xi^2}[p+\sqrt{p^2-\xi^2}]^{2n}} = \frac{1}{\sqrt{p^2-\xi^2}}\left[\frac{p}{\xi} - \sqrt{\frac{p^2}{\xi^2}-1}\right]^{2n}. \tag{64}$$

Now, as far as the imaginary part of $\widetilde{\mathcal{Y}}_{2n,0}(\xi)$ is concerned, in the expansion of (64), the relevant terms come from those which are of even order in ξ, and thus of even order in the square root factor in the numerator. We thus recognize the relevant terms as

$$\frac{1}{\sqrt{p^2-\xi^2}}\sum_{l=0}^{n}{}^{2n}C_{2l}\left(\frac{p}{\xi}\right)^{2n-2l}\left(\frac{p^2}{\xi^2}-1\right)^{l} = \frac{(-1)^n}{\sqrt{p^2-\xi^2}}\cos\left[2n\arcsin\left(\frac{p}{\xi}\right)\right], \tag{65}$$

where ${}^{2n}C_{2l}$ denotes a binomial coefficient. Hence, we obtain

$$\mathrm{Im}[\widetilde{\mathcal{Y}}_{2n,0}(\xi)] = \frac{1}{\pi}\sum_{p=1}^{\lfloor\xi\rfloor}\frac{1}{\sqrt{\xi^2-p^2}}\cos\left[2n\arcsin\left(\frac{p}{\xi}\right)\right]. \tag{66}$$

This enables us to generalize (16) and (56) to arbitrary order $2n$, $n \geqslant 0$, that is (see also [10])

$$\mathcal{G}_{2n,0}(\xi) = \sum_{h=1}^{\infty}J_{2n}(2\pi\xi h) = \frac{1}{2\pi\xi} - \frac{1}{2}\delta_{n,0} + \mathrm{Im}[\widetilde{\mathcal{Y}}_{2n,0}(\xi)]. \tag{67}$$

5. Conclusions

The expressions we have given for a general class of Bessel functions have been shown to be numerically efficient and flexible. They could be extended to take into account position-dependent phase factors of the type associated with off-axis beams incident upon gratings, but the formulae here cover the most important case of normal incidence. The fact that the formulae work remarkably well for large values of the parameter ξ, all the involved series showing an exponential convergence, means that multipole Green's function expressions should be able to be used for periodic problems incorporating supercells with hundreds or even thousands of elements, as we hope to demonstrate in future work.

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Appendix

There is an interesting connection between the grating sums evaluated in (12) and (44) and density of state functions. The latter are important in solid-state physics, being connected for example with the evaluation of specific heat of crystalline solids or the radiation properties of sources in photonic crystals. The connection we will exhibit is for the two-dimensional density of states associated with free space, subject to the condition of one-dimensional periodicity associated with a grating. In situations where the grating has cylinders at each integer point, the density of states becomes dependent on a position vector $\mathbf{r}$, as well as on the angular frequency ω, and is written as $\rho(\omega, \mathbf{r})$. Here, the cylinders have infinitesimal radius or refractive index of unity, and so the density of states function becomes independent of $\mathbf{r}$, but we will retain the customary notation for ρ.

The density of states is given by [13]

$$\rho(\omega, \mathbf{r}) = -\frac{2\omega}{\pi c^2} \operatorname{Im}[G^+(\omega, \mathbf{r} = \mathbf{r}')], \tag{A.1}$$

where G^+ is the appropriate Green's function, given in its spatial representation, and putting $\mathbf{r} - \mathbf{r}' = (x, y)$, by

$$G^+(\omega, x, y) = -\frac{\mathrm{i}}{4} \sum_{n=-\infty}^{\infty} H_0^{(1)}\left[\frac{\omega}{c}\sqrt{(x-n)^2 + y^2}\right]. \tag{A.2}$$

The sum over Hankel functions is expanded using Graf's addition theorem [9] for $x^2 + y^2 < 1$, and becomes

$$G^+(\omega, x, y) = -\frac{\mathrm{i}}{4}\left[(1 + S_0(\omega)) J_0\left(\frac{\omega}{c}\sqrt{x^2+y^2}\right) + \mathrm{i}Y_0\left(\frac{\omega}{c}\sqrt{x^2+y^2}\right)\right.$$
$$\left. + 2\sum_{\ell=1}^{\infty} S_{2\ell}(\omega) J_{2\ell}\left(\frac{\omega}{c}\sqrt{x^2+y^2}\right)\right]. \tag{A.3}$$

Here the $S_\ell(\omega)$ denote sums of Hankel functions over the grating, of which only the zeroth order sum is needed here:

$$S_0(\omega) = S_0^J(\omega) + \mathrm{i}S_0^Y(\omega) = 2\left[\sum_{n=1}^{\infty} J_0\left(\frac{n\omega}{c}\right) + \mathrm{i}\sum_{n=1}^{\infty} Y_0\left(\frac{n\omega}{c}\right)\right]. \tag{A.4}$$

By substituting (41) and (45), with the corresponding arguments, into (A.4), we may write (A.4) as

$$S_0(\omega) = -1 + \frac{2c}{\omega} + 2\mathrm{i}\overline{\widetilde{\mathcal{Y}}}_{0,0}\left(\frac{\omega}{2\pi c}\right), \tag{A.5}$$

where the superposed bar denotes complex conjugation. Then, using (A.3) in (A.1), we find

$$\rho(\omega, \mathbf{r}) = \frac{\omega}{2\pi c^2}\{1 + \mathrm{Re}[S_0(\omega)]\} = \frac{1}{\pi c}\left\{1 + \frac{\omega}{c}\,\mathrm{Im}\left[\widetilde{\mathcal{Y}}_{0,0}\left(\frac{\omega}{2\pi c}\right)\right]\right\}. \tag{A.6}$$

Comparing (A.6) with (45), we see that the right-hand side of (45) has a physical significance, while the terms coming from (12) and (44) do not have a physical significance when they are separate. Combining (A.6) with (44), we obtain the density of states function:

$$\rho(\omega, \mathbf{r}) = \frac{1}{\pi c}\left[1 + 2\sum_{n=1}^{\lfloor \omega/2\pi c\rfloor} \frac{1}{\sqrt{1 - (4\pi^2 c^2 n^2/\omega^2)}}\right]. \tag{A.7}$$

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