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# Efficient calculation of the Green's function for electromagnetic scattering by gratings

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We consider both the spatial domain and spectral domain forms of the Green's function, appropriate in the electromagnetic diffraction of a plane wave incident in the $xy$ plane on a singly periodic structure, or grating, oriented along the $x$ axis. For the spectral domain form, we exhibit, for an obliquely incident plane wave, cubically convergent forms for the Green's function and both its $x$ and $y$ derivatives. We compare the spatial and spectral forms of the Green's function, and so establish expressions from which grating lattice sums can be efficiently evaluated for normal incidence. We use these lattice sums in an alternative expression for the Green's function, which we show to be computationally faster than the accelerated spectral domain expressions for the Green's function if knowledge of this function at several points is required, for small values of $y$.

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## I. INTRODUCTION

The calculation of the free-space Green's function in problems of electromagnetic diffraction by singly periodic structures (gratings) is the key to the efficient numerical solution of many current questions of technological importance. Important work on this question has been carried out by Maystre [1,2] and Tayeb [3]. Recent studies have discussed means of achieving accurate and efficient evaluations of the two important forms used for the Green's function—the spatial and spectral representations [4–8].

The spatial form represents the Green's function as a sum of fields radiated by a sum of appropriately phased line sources, and so writes the solution of the Helmholtz equation in terms of Hankel functions multiplied by trigonometric angular dependencies. The spectral form represents the Green's function as a sum of plane waves, each obeying the appropriate quasiperiodicity condition [9]. Each of these forms is slowly convergent, and so numerical and analytic strategies have to be devised to enhance the convergence of the series if prohibitive computation times are to be avoided.

In the past, the strategies adopted to accelerate convergence [4–8] have relied on several ideas. Kummer's transformation has been used to subtract off an analytically summable series, leaving a more rapidly convergent series to be summed numerically. Poisson's summation formula has been used to transform a slowly convergent series in the spatial domain into a more rapidly convergent series in the spectral domain, and vice versa. Also, algorithms such as those of Shanks [10] and Wynn [11] have been used to accelerate the convergence of oscillating and monotonic series.

Here, we start by considering the spectral Green's function for the case of a plane wave incident, in the $xy$ plane, at an arbitrary angle on a grating along the $x$ axis, and accelerate its convergence by using Kummer's transformation. We show how, in principle, the series may be made convergent to an arbitrary order, and exhibit forms which are quadratically, cubically and fourth-order convergent. The last forms are derived because they yield cubically convergent forms for the spatial derivatives of the Green's function.

Next, we compare the spectral and spatial forms of the Green's function. We expand the resultant identity using Graf's addition theorem, and we compute the lattice sums for the case of normally incident radiation. The case of arbitrary incidence and quasiperiodicity [9] is considerably more complex, and so it will be discussed in later work. These lattice sums have only been evaluated hitherto for the sum of zeroth order; here, we exhibit a recurrence formula which enables their calculation to arbitrarily high order. We use the lattice sums to construct an alternative expression for the Green's function, which we show to converge sufficiently rapidly to justify its use over other techniques in situations where the Green's function $G(x,y)$ has to be evaluated for small values of $y$. (The lattice sums are independent of the point at which the field is evaluated, and therefore the time penalty in calculating them is amortized over the number of Green's function evaluations.)

We present numerical results confirming our results in both graphical and tabular form, in order to aid those wishing to implement our methods. For the same reason, we give in an Appendix formulas which may be used to rapidly evaluate the less common transcendental functions used in our analysis.

The derivations presented here are in some cases complicated, and involve a range of special functions. However, our results are readily computable (and we are prepared to give interested readers copies of our MATHEMAT-

 

ICA programs for them). For readers more interested in results than derivations, our key equations are (10), (11), (39), and (43), while Table II may provide motivation to those bogged down in a quagmire of analysis.

## II. THIRD-ORDER ACCELERATION OF SERIES CONVERGENCE

### A. Plane wave expansion of the Green's function

In grating problems, for a fixed incidence angle $\theta$ and period $d$, we are led to consider a Green's function $G(x,y)$ which obeys the inhomogeneous Helmholtz equation:

$$(\nabla^2 + k^2)G(x,y) = \delta(y) \sum_{n=-\infty}^{\infty} \delta(x-nd)e^{i\alpha_0 nd} , \tag{1}$$

where $\alpha_0 \stackrel{\text{def}}{=} k\sin\theta$ and $k$ is the wave number of the incident plane wave.

This function $G$ is given by one or the other of the following forms usually called the "spatial form" and the "spectral form [5]." We will denote these two forms by $G_d$ and $G_r$, respectively. If $H_0^{(1)}$ stands for the zeroth-order Hankel function of the first kind, the spatial form is

$$G_d(x,y) = \frac{1}{4i} \sum_{n=-\infty}^{\infty} H_0^{(1)}[k\sqrt{(x-nd)^2+y^2}]\, e^{i\alpha_0 nd}. \tag{2}$$

The spectral form, which is linked to the spatial form using the Fourier transform, is

$$G_r(x,y) = \frac{1}{2id} \sum_{n=-\infty}^{\infty} \frac{1}{\chi_n}\, e^{i(\alpha_n x + \chi_n |y|)}, \tag{3}$$

where

$$\alpha_n = \alpha_0 + nK = \alpha_0 + \frac{2\pi n}{d} ,$$
$$\chi_n = \begin{cases} \sqrt{k^2-\alpha_n^2} \; , & \alpha_n^2 \le k^2 \\ i\sqrt{\alpha_n^2 - k^2} \; , & \alpha_n^2 > k^2 \; . \end{cases} \tag{4}$$

The series (3) may be written in the form

$$G_r(x,y) = \frac{e^{i\alpha_0 x}}{2d} \left\{ \frac{e^{i\chi_0|y|}}{i\chi_0} + S(x,y) \right\} . \tag{5}$$

Here, we have denoted by $S(x,y)$ the series

$$S(x,y) = \sum_{n\in\mathcal{Z}^*} \frac{e^{i\chi_n|y|}}{i\chi_n}\, e^{inKx} \tag{6}$$

and $\mathcal{Z}^* = \mathcal{Z} \setminus \{0\}$. We apply the Kummer method for series acceleration [12]; i.e., we subtract and add to (6) its asymptotic form, summing the asymptotic form analytically. To evaluate the asymptotic behavior of $S(x,y)$, for large $n$, we consider the expansions (readily verified by *Mathematica*):

$$\begin{aligned}\chi_n &= i\,|\alpha_n|\,\sqrt{1-(k/\alpha_n)^2} \\ &= i\left\{ |n|K + \alpha_0\,\mathrm{sgn}(n) - \frac{k^2}{2|n|K} + \frac{\alpha_0 k^2}{2n|n|K^2} \right. \\ &\quad \left. - \frac{k^2(\alpha_0^2 + k^2/4)}{2n^2|n|K^3} + O\left(\frac{1}{n^4}\right) \right\} ,\end{aligned}$$

$$\frac{1}{i\chi_n} = -\frac{1}{|n|K} + \frac{\alpha_0}{n|n|K^2} - \frac{\alpha_0^2 + k^2/2}{n^2|n|K^3} + O\left(\frac{1}{n^4}\right) .$$

We keep only terms of order $1/n^2$, such that the general term in (6) has the asymptotic form

$$\begin{aligned}\frac{e^{i\chi_n|y|}}{i\chi_n}\, e^{inKx} &\sim e^{-\{|n|K+\alpha_0\,\mathrm{sgn}(n) - k^2/(2|n|K)\}|y|} \\ &\quad \times \left[ -\frac{1}{|n|K} + \frac{\alpha_0}{n|n|K^2} \right] e^{inKx},\end{aligned} \tag{7}$$

and, for large $n$, we expand

$$e^{k^2|y|/(2|n|K)} = 1 + \frac{k^2|y|}{2|n|K} + O\left(\frac{1}{n^2}\right) .$$

Neglecting the terms of order higher than $1/n^2$, we obtain

$$\begin{aligned}\frac{e^{i\chi_n|y|}}{i\chi_n} &\approx \frac{e^{-\{|n|K+\alpha_0\,\mathrm{sgn}(n)\}|y|}}{|n|K} \left[ -1 + \frac{\alpha_0}{nK} - \frac{k^2|y|}{2|n|K} \right] \\ &\equiv u_n(y) \; .\end{aligned} \tag{8}$$

The sum of the asymptotic series

$$S_a(x,y) = \sum_{n\in\mathcal{Z}^*} u_n(y)\, e^{inKx} \tag{9}$$

can be put in closed form using appropriate, but exotic, special functions:

$$\begin{aligned} S_a(x,y) &= e^{-\alpha_0|y|} \sum_{n=1}^{\infty} \frac{e^{nK(-|y|+ix)}}{nK} \left( -1 + \frac{\alpha_0}{nK} - \frac{k^2|y|}{2nK} \right) + e^{\alpha_0|y|} \sum_{n=1}^{\infty} \frac{e^{nK(-|y|-ix)}}{nK} \left( -1 - \frac{\alpha_0}{nK} - \frac{k^2|y|}{2nK} \right) \\ &= e^{-\alpha_0|y|} \left\{ \frac{1}{K} \ln(1 - e^{-K|y|+iKx}) + \frac{1}{K^2} \left( \alpha_0 - \frac{k^2|y|}{2} \right) \mathrm{Li}_2(e^{-K|y|+iKx}) \right\} \\ &\quad + e^{\alpha_0|y|} \left\{ \frac{1}{K} \ln(1 - e^{-K|y|-iKx}) - \frac{1}{K^2} \left( \alpha_0 + \frac{k^2|y|}{2} \right) \mathrm{Li}_2(e^{-K|y|-iKx}) \right\}. \end{aligned} \tag{10}$$

Here, $\mathrm{Li}_2$ is the dilogarithm function (see Appendix) and we have used the relation [12]

$$\sum_{n=1}^{\infty} \frac{z^n}{n} = -\ln(1-z), \ |z| \le 1,$$

which holds true even if $|z| = 1$, provided that $z$ is not precisely unity [13].

Finally, the Green's function (5) may be written in the form

$$G_r(x,y) = \frac{e^{i\alpha_0 x}}{2d}\left\{\frac{e^{i\chi_0|y|}}{i\chi_0} + S_a(x,y) + \sum_{n\in\mathcal{Z}^*} e^{inKx} \times \left[\frac{e^{i\chi_n|y|}}{i\chi_n} + \frac{e^{-\{|n|K+\alpha_0\,\mathrm{sgn}(n)\}|y|}}{|n|K} \times \left(1 - \frac{\alpha_0}{nK} + \frac{k^2|y|}{2|n|K}\right)\right]\right\}, \tag{11}$$

containing a series which converges as

$$\sim e^{-|ny|K}\, O\left(\frac{1}{n^3}\right).$$

## B. First-order derivatives of the Green's function

In order to obtain the same rate of convergence for the first-order derivatives of Green's function (5), with respect to $x$ and $y$, we need a Green's function represented by series converging as $\sim e^{-|ny|K} O(1/n^4)$. This means repeating the above method taking into account terms of order $1/n^3$. To allow a comparison of numerical results, we will give here the final expressions of the first-order derivatives of Green's function, in terms of series converging as $1/n^3$. In this case, (8) takes the form

$$\frac{e^{i\chi_n|y|}}{i\chi_n} \approx \frac{e^{-\{|n|K+\alpha_0 \mathrm{sgn}(n)\}|y|}}{|n|K} \times \left[-1 + \frac{\alpha_0}{nK} - \frac{k^2|y|}{2|n|K} + \frac{\alpha_0 k^2|y|}{n|n|K^2} - \frac{8\alpha_0^2 + 4k^2 + k^4y^2}{8n^2K^2}\right] \equiv w_n(y)\ . \tag{12}$$

Consequently, we obtain

$$S_a(x,y) = e^{-\alpha_0|y|}\left\{\frac{1}{K}\ln\left(1 - e^{-K|y|+iKx}\right) + \frac{1}{K^2}\left(\alpha_0 - \frac{k^2|y|}{2}\right)\mathrm{Li}_2\left(e^{-K|y|+iKx}\right) + \frac{1}{K^3}\left(\alpha_0 k^2|y| - \frac{8\alpha_0^2 + 4k^2 + k^4y^2}{8}\right)\mathrm{Li}_3\left(e^{-K|y|+iKx}\right)\right\}$$
$$+ e^{\alpha_0|y|}\left\{\frac{1}{K}\ln\left(1 - e^{-K|y|-iKx}\right) - \frac{1}{K^2}\left(\alpha_0 + \frac{k^2|y|}{2}\right)\mathrm{Li}_2\left(e^{-K|y|-iKx}\right) - \frac{1}{K^3}\left(\alpha_0 k^2|y| + \frac{8\alpha_0^2 + 4k^2 + k^4y^2}{8}\right)\mathrm{Li}_3\left(e^{-K|y|+iKx}\right)\right\}, \tag{13}$$

where $\mathrm{Li}_3$ is the trilogarithm function (see Appendix), and the Green's function is

$$G_r(x,y) = \frac{e^{i\alpha_0 x}}{2d}\left\{\frac{e^{i\chi_0|y|}}{i\chi_0} + S_a(x,y) + \sum_{n\in\mathcal{Z}^*} e^{inKx}\left[\frac{e^{i\chi_n|y|}}{i\chi_n} - w_n(y)\right]\right\}\ . \tag{14}$$

The first-order derivatives of the Green's function are given by the formulas

$$\frac{\partial G_r}{\partial x} = i\alpha_0\, G_r(x,y) + \frac{e^{i\alpha_0 x}}{2d}\left\{\frac{\partial S_a}{\partial x} + iK\sum_{n\in\mathcal{Z}^*} n\, e^{inKx}\left[\frac{e^{i\chi_n|y|}}{i\chi_n} - w_n(y)\right]\right\}\ , \tag{15}$$

$$\frac{\partial G_r}{\partial y} = \mathrm{sgn}\,(y)\ \frac{e^{i\alpha_0 x}}{2d}\left\{e^{i\chi_0|y|} + \frac{\partial S_a}{\partial|y|} + \sum_{n\in\mathcal{Z}^*} e^{inKx}\left[e^{i\chi_n|y|} - \frac{\partial w_n}{\partial|y|}\right]\right\}\ , \tag{16}$$

where the series converge as $\sim e^{-|ny|K}O(1/n^3)$. Here,

$$\frac{\partial S_a}{\partial x} = -ie^{-\alpha_0|y|}\left\{(e^{K|y|-iKx}-1)^{-1} + \frac{1}{K}\left(\alpha_0 - \frac{k^2|y|}{2}\right)\ln(1-e^{-K|y|+iKx}) - \frac{1}{K^2}\left(\alpha_0 k^2|y| - \frac{8\alpha_0^2+4k^2+k^4y^2}{8}\right)\mathrm{Li}_2(e^{-K|y|+iKx})\right\}$$
$$+ie^{\alpha_0|y|}\left\{(e^{K|y|+iKx}-1)^{-1} - \frac{1}{K}\left(\alpha_0 + \frac{k^2|y|}{2}\right)\ln(1-e^{-K|y|-iKx}) + \frac{1}{K^2}\left(\alpha_0 k^2|y| + \frac{8\alpha_0^2+4k^2+k^4y^2}{8}\right)\mathrm{Li}_2(e^{-K|y|-iKx})\right\},$$

$$\frac{\partial S_a}{\partial |y|} = e^{-\alpha_0|y|}\left\{(e^{K|y|-iKx}-1)^{-1} - \frac{k^2|y|}{2K}\ln(1-e^{-K|y|+iKx}) + \frac{k^2|y|}{2K^2}\left(-\alpha_0 + \frac{k^2|y|}{4}\right)\mathrm{Li}_2(e^{-K|y|+iKx}) + \frac{1}{K^3}\left[\alpha_0^3 + \frac{3\alpha_0 k^2}{2} - k^2\left(\alpha_0^2+\frac{k^2}{4}\right)|y| + \frac{\alpha_0 k^4 y^2}{8}\right]\mathrm{Li}_3(e^{-K|y|+iKx})\right\}$$
$$+e^{\alpha_0|y|}\left\{(e^{K|y|+iKx}-1)^{-1} - \frac{k^2|y|}{2K}\ln(1-e^{-K|y|-iKx}) + \frac{k^2|y|}{2K^2}\left(\alpha_0 + \frac{k^2|y|}{4}\right)\mathrm{Li}_2(e^{-K|y|-iKx}) - \frac{1}{K^3}\left[\alpha_0^3 + \frac{3\alpha_0 k^2}{2} + k^2\left(\alpha_0^2+\frac{k^2}{4}\right)|y| + \frac{\alpha_0 k^4 y^2}{8}\right]\mathrm{Li}_3(e^{-K|y|-iKx})\right\},$$

$$\frac{\partial w_n}{\partial |y|} = e^{-\{|n|K+\alpha_0\mathrm{sgn}(n)\}|y|}\left\{1 + \frac{k^2|y|}{2|n|K} - \frac{k^2}{2(|n|K)^2}\left[\alpha_0\mathrm{sgn}(n)|y| - \frac{k^2y^2}{4}\right] + \frac{1}{(|n|K)^3}\left[\alpha_0\mathrm{sgn}(n)\left(\alpha_0^2+\frac{3k^2}{2}\right) - \left(\alpha_0^2+\frac{k^2}{4}\right)k^2|y| + \alpha_0\mathrm{sgn}(n)\frac{k^4y^2}{8}\right]\right\}.$$

## III. NORMAL INCIDENCE: PERIODIC GREEN'S FUNCTION

### A. Lattice sums

From now on, we shall be concerned only with the study of gratings in normal incidence. In this case ($\alpha_0 = 0$ and $\alpha_n = nK$), we will obtain some formulas of practical interest by equating the spatial form (2) and the spectral form (3) of the Green's function. Using these formulas we will be able to compute accurately the so-called lattice sums which, as proved below, allow us to reduce the computation time when, in a certain problem, the Green's function has to be evaluated at a large number of points (perhaps as many as several hundreds). We confess that the involved mathematics are tedious and cumbersome but, as we will show in Sec. IV, the result is worth the effort. By assuming $y = 0$ but $x \neq 0$, and equating (2) and (3) we obtain

$$\sum_{n\in\mathcal{Z}} H_0^{(1)}(k|x-nd|) = \frac{2}{d}\sum_{n\in\mathcal{Z}}\frac{1}{\chi_n}\,e^{i\alpha_n x} \tag{17}$$

or, for $x \geq 0$,

$$H_0^{(1)}(kx) + \sum_{n\in\mathcal{Z}^*} H_0^{(1)}(k|x-nd|) = \frac{2}{d}\sum_{n\in\mathcal{Z}}\frac{1}{\chi_n}e^{i\alpha_n x}. \tag{18}$$

In (18) we apply the addition theorem for Bessel functions [12], for $-d < x < d$ so that $|nd| > |x|$, $\forall n \neq 0$:

$$H_0^{(1)}(kx) + \sum_{n\in\mathcal{Z}^*}\sum_{\ell=-\infty}^{\infty} H_\ell^{(1)}(k|n|d)\, e^{i\ell\varphi_n}\, J_\ell(kx)e^{-i\ell\theta_x} = \frac{2}{d}\sum_{n\in\mathcal{Z}}\frac{1}{\chi_n}\, e^{i\alpha_n x}. \tag{19}$$

Here, $\theta_x = \pi H(-x)$ and $\varphi_n = \pi H(-n)$, where $H$ is the Heaviside step function:

$$H(x) = \begin{cases} 0 \text{ if } x < 0 \\ 1 \text{ if } x > 0. \end{cases}$$

For $k$ and $d$ fixed, let us call *lattice sum of order* $\ell$ the complex number $S_\ell(k,d)$, defined as

$$S_\ell(k,d) = \sum_{n\in\mathcal{Z}^*} H_\ell^{(1)}(n|k|d)\, e^{i\ell\varphi_n}. \quad (20)$$

With this notation, (19) becomes (for $x > 0$ we have $\theta_x = 0$) [14]

$$H_0^{(1)}(kx) + \sum_{\ell=-\infty}^{\infty} S_\ell(k,d) J_\ell(kx) = \frac{2}{d}\sum_{n\in\mathcal{Z}} \frac{1}{\chi_n} e^{i\alpha_n x}. \quad (21)$$

From (20) we deduce that, for normal incidence, the lattice sums of odd order vanish. Taking into account that $\varphi_n = 0$ for $n > 0$ and $\varphi_n = \pi$ for $n < 0$, we obtain

$$\begin{aligned} S_\ell(k,d) &= \sum_{n=1}^{\infty}\{[J_\ell(nkd) + iY_\ell(nkd)] \\ &\quad + [J_\ell(nkd) + iY_\ell(nkd)]\exp(i\ell\pi)\} \\ &= \sum_{n=1}^{\infty}\{J_\ell(nkd)[1 + (-1)^\ell] \\ &\quad + iY_\ell(nkd)[1 + (-1)^\ell]\}. \end{aligned}$$

If we define $S_\ell^J(k,d)$ and $S_\ell^Y(k,d)$ as the real and imaginary part of $S_\ell(k,d)$, respectively, then

$$S_{2\ell}^J(k,d) = 2\sum_{n=1}^{\infty} J_{2\ell}(nkd), \quad S_{2\ell+1}^J(k,d) = 0,$$

$$S_{2\ell}^Y(k,d) = 2\sum_{n=1}^{\infty} Y_{2\ell}(nkd), \quad S_{2\ell+1}^Y(k,d) = 0\ ,$$

and (21) takes the form

$$H_0^{(1)}(kx) + S_0(k,d)J_0(kx) + 2\sum_{\ell=1}^{\infty} S_{2\ell}(k,d)J_{2\ell}(kx) = \frac{2}{d}\sum_{n\in\mathcal{Z}} \frac{1}{\chi_n} e^{i\alpha_n x}. \quad (22)$$

Assuming that $k/K$ is not an integer, we say that $n \in \Omega$ or $n \in \overline{\Omega}$ depending whether $k^2 - n^2K^2$ is positive or negative. We decompose $\Omega$ in three subsets: $\Omega^+$ ($n > 0$), $\Omega^-$ ($n < 0$), and $\{0\}$. In the same way, $\overline{\Omega}$ is decomposed in $\overline{\Omega^+}$ ($n > 0$) and $\overline{\Omega^-}$ ($n < 0$). With these notations, the right hand side of (22) may be written in the form

$$\begin{aligned} \sum_{n\in\mathcal{Z}} \frac{1}{\chi_n}\, e^{i\alpha_n x} &= \sum_{n\in\Omega} \frac{1}{\chi_n}\, e^{i\alpha_n x} + \sum_{n\in\overline{\Omega}} \frac{1}{i|\chi_n|}\, e^{i\alpha_n x} \\ &= \sum_{n\in\Omega} \frac{1}{\chi_n}\, e^{i\alpha_n x} + \sum_{n\in\overline{\Omega}^-} \frac{1}{i|\chi_n|}\, e^{i\alpha_n x} + \sum_{n\in\overline{\Omega}^+} \frac{1}{i|\chi_n|}\, e^{i\alpha_n x} \\ &= \frac{1}{k} + \sum_{n\in\Omega^+} \frac{\exp(i\alpha_n x) + \exp(-i\alpha_n x)}{\chi_n} + \sum_{n\in\overline{\Omega}^+} \frac{\exp(i\alpha_n x) + \exp(-i\alpha_n x)}{i|\chi_n|} \\ &= \frac{1}{k} + 2\sum_{n\in\Omega^+} \frac{\cos(\alpha_n x)}{\chi_n} + 2\sum_{n\in\overline{\Omega}^+} \frac{\cos(\alpha_n x)}{i|\chi_n|}\ . \end{aligned}$$

Substituting in (22) and equating the real and imaginary parts we obtain the equations

$$J_0(kx) + S_0^J(k,d)J_0(kx) + 2\sum_{\ell=1}^{\infty} S_{2\ell}^J(k,d)J_{2\ell}(kx) = \frac{2}{d}\left\{\frac{1}{k} + 2\sum_{n\in\Omega^+} \frac{\cos(\alpha_n x)}{\chi_n}\right\}, \quad (23)$$

$$Y_0(kx) + S_0^Y(k,d)J_0(kx) + 2\sum_{\ell=1}^{\infty} S_{2\ell}^Y(k,d)J_{2\ell}(kx) = -\frac{4}{d}\sum_{n\in\overline{\Omega}^+} \frac{\cos(\alpha_n x)}{|\chi_n|}. \quad (24)$$

In the first equation, $\alpha_n < k$, $\forall n \in \Omega^+$. Consequently, the general solution is obtained by substituting, in the right hand side, the Jacobi expansion [12]:

$$\begin{aligned} \cos(\alpha_n x) &= \cos\{kx \sin[\arcsin(\alpha_n/k)]\} \\ &= J_0(kx) + 2\sum_{\ell=1}^{\infty} J_{2\ell}(kx) \\ &\quad \times \cos[2\ell \arcsin(\alpha_n/k)]. \end{aligned}$$

By equating the coefficients of the corresponding Bessel functions we obtain the general solution of (23) in the form [15,16]:

$$S^J_{2\ell}(k,d) = 2\sum_{m=1}^{\infty} J_{2\ell}(mkd)$$

$$= -\delta_{\ell,0} + \frac{2}{kd} + \frac{4}{d}\sum_{n\in\Omega^+} \frac{\cos\left[2\ell\arcsin\left(\alpha_n/k\right)\right]}{\sqrt{k^2-\alpha_n^2}}. \quad (25)$$

Note that the restriction $n \in \Omega^+$ implies a finite sum, not a series.

On the other hand substituting the Neumann series [12]

$$Y_0(kx) = \frac{2}{\pi}\left[\ln\left(\frac{kx}{2}\right)+\gamma\right]J_0(kx) - \frac{4}{\pi}\sum_{\ell=1}^{\infty}\frac{(-1)^\ell}{\ell}J_{2\ell}(kx) \quad (26)$$

in Eq. (24), we obtain

$$\left\{S_0^Y(k,d) + \frac{2}{\pi}\left[\ln\left(\frac{kx}{2}\right)+\gamma\right]\right\}J_0(kx) + 2\sum_{\ell=1}^{\infty}\left[S_{2\ell}^Y(k,d) - \frac{2}{\pi}\frac{(-1)^\ell}{\ell}\right]J_{2\ell}(kx) = -\frac{4}{d}\sum_{n\in\overline{\Omega}^+}\frac{\cos\left(\alpha_n x\right)}{|\chi_n|}, \quad (27)$$

where $\gamma = 0.577216$ is the Euler-Mascheroni constant.

In the zeroth-order approximation, with respect to $x$, the right hand side of (27) becomes

$$-\frac{4}{d}\sum_{n\in\overline{\Omega}^+}\frac{\cos\left(\alpha_n x\right)}{|\chi_n|} \approx -\frac{4}{d}\left\{\sum_{n\in\overline{\Omega}^+}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right] - \sum_{n\in\Omega^+}\frac{1}{\alpha_n}\right\} + \frac{2}{\pi}\ln\left(Kx\right). \quad (28)$$

Here, we have used the asymptotic form

$$\frac{1}{|\chi_n|} = \frac{1}{\alpha_n\sqrt{1-(k/\alpha_n)^2}} \sim \frac{1}{\alpha_n} \quad \text{as } n\to\infty\ , \quad (29)$$

and we have applied Kummer's transformation for series acceleration, so that

$$\sum_{n\in\overline{\Omega}^+}\frac{\cos\left(\alpha_n x\right)}{|\chi_n|} = \sum_{n\in\overline{\Omega}^+}\cos\left(\alpha_n x\right)\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right] + \sum_{n\in\overline{\Omega}^+}\frac{\cos\left(\alpha_n x\right)}{\alpha_n}$$
$$= \sum_{n\in\overline{\Omega}^+}\cos\left(\alpha_n x\right)\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right] - \sum_{n\in\Omega^+}\frac{\cos\left(\alpha_n x\right)}{\alpha_n} + \sum_{n=1}^{\infty}\frac{\cos\left(\alpha_n x\right)}{\alpha_n}.$$

For small $x$, in the first two terms, we use the approximations $\cos(\alpha_n x) \approx 1$. At the same time, if $0 < Kx < 2\pi$ (i.e., $0 < x < d$), the last series has a closed-form sum [12]

$$\sum_{n=1}^{\infty}\frac{\cos\left(\alpha_n x\right)}{\alpha_n} = \frac{1}{K}\sum_{n=1}^{\infty}\frac{\cos\left(nKx\right)}{n} = -\frac{1}{K}\ln\left(2\sin\frac{Kx}{2}\right) \approx -\frac{1}{K}\ln\left(Kx\right)\ . \quad (30)$$

Finally, for small $x$, $J_0(kx) \approx 1$, $J_{2\ell}(kx) \approx 0$ ($\ell \geq 1$) and, from (27,28), we obtain the expression [16,17]

$$S_0^Y(k,d) = -\frac{2}{\pi}\left[\ln\left(\frac{k}{2K}\right)+\gamma\right] - \frac{4}{d}\left\{\sum_{n\in\overline{\Omega}^+}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right] - \sum_{n\in\Omega^+}\frac{1}{\alpha_n}\right\}. \quad (31)$$

This represents $S_0^Y$ in terms of a quadratically convergent series.

To obtain the lattice sums of higher orders we substitute the expression of $S_0^Y$ in (27), then we consider the series expansions of the Bessel functions up to the order $2\ell$. The coefficient of $x^{2\ell}$, in the left hand side of (27), is given by the formula

$$2\sum_{j=1}^{\ell}\left[S_{2j}^Y - \frac{2}{\pi}\cdot\frac{(-1)^j}{j}\right](-1)^{\ell-j}\frac{(k/2)^{2\ell}}{(\ell-j)!(\ell+j)!} - \frac{4}{d}\left\{\sum_{n\in\overline{\Omega}^+}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right] - \sum_{n\in\Omega^+}\frac{1}{\alpha_n}\right\} \times(-1)^\ell\frac{(k/2)^{2\ell}}{(\ell!)^2} + \frac{2}{\pi}(-1)^\ell\frac{(k/2)^{2\ell}}{(\ell!)^2}\ln\left(Kx\right). \quad (32)$$

In the right hand side of (27) we consider, instead of the asymptotic form of $1/|\chi_n|$, its Taylor expansion up to the order $\ell$:

$$\frac{1}{|\chi_n|} = \frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0) + O\left(\frac{1}{n^{2\ell+1}}\right),$$

where $P_{2s}$ represents the Legendre polynomials. Kummer's method leads us to the expressions

$$-\frac{4}{d}\left\{\sum_{n\in\overline{\Omega}^+}\cos(\alpha_n x)\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right]+\sum_{n\in\overline{\Omega}^+}\frac{\cos(\alpha_n x)}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right\}$$

$$=-\frac{4}{d}\left\{\sum_{n\in\overline{\Omega}^+}\cos(\alpha_n x)\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right]\right.$$
$$\left.-\sum_{n\in\Omega^+}\frac{\cos(\alpha_n x)}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right\}-\frac{4}{d}\sum_{n=1}^{\infty}\frac{\cos(\alpha_n x)}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)$$
$$=-\frac{4}{d}\left\{\sum_{n\in\overline{\Omega}^+}\cos(\alpha_n x)\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right]\right.$$
$$\left.-\sum_{n\in\Omega^+}\frac{\cos(\alpha_n x)}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right\}-\frac{2}{\pi}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{K}\right)^{2s}P_{2s}(0)Cl_{2s+1}(Kx). \quad (33)$$

Here, $\mathrm{Cl}_{2s+1}$ is the generalized Clausen function (see Appendix).

Now, we substitute (A6) in (33) and expand the cosine functions in power series. The coefficient of $x^{2\ell}$ is given by

$$-\frac{(-1)^\ell}{(2\ell)!}\frac{4}{d}\left\{\sum_{n\in\overline{\Omega}^+}\alpha_n^{2\ell}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right]-\sum_{n\in\Omega^+}\frac{\alpha_n^{2\ell}}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right\}$$
$$+\frac{2}{\pi}\frac{k^{2\ell}}{(2l)!}P_{2\ell}(0)\ln(Kx)-\frac{2}{\pi}\frac{k^{2\ell}}{(2\ell)!}P_{2\ell}(0)\left(\sum_{p=1}^{2\ell}\frac{1}{p}\right)+(-1)^\ell\frac{2}{\pi}\frac{K^{2\ell}}{(2\ell)!}\sum_{s=0}^{\ell-1}(-1)^s\left(\frac{k}{K}\right)^{2s}P_{2s}(0)\frac{B_{2\ell-2s}}{(2\ell-2s)}. \quad (34)$$

Substituting

$$P_{2s}(0)=(-1)^s\frac{(2s-1)!!}{2^s\, s!}=(-1)^s\frac{(2s)!}{2^{2s}\,(s!)^2}$$

in the last three terms of (34), we obtain

$$-\frac{(-1)^\ell}{(2\ell)!}\frac{4}{d}\left\{\sum_{n\in\overline{\Omega}^+}\alpha_n^{2\ell}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right]-\sum_{n\in\Omega^+}\frac{\alpha_n^{2\ell}}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right\}$$
$$+\frac{2}{\pi}(-1)^\ell\frac{(k/2)^{2\ell}}{(\ell!)^2}\ln(Kx)-\frac{2}{\pi}(-1)^\ell\frac{(k/2)^{2\ell}}{(\ell!)^2}\left(\sum_{p=1}^{2\ell}\frac{1}{p}\right)+\frac{2}{\pi}(-1)^\ell\frac{K^{2\ell}}{(2\ell)!}\sum_{s=0}^{\ell-1}\left(\frac{k}{2K}\right)^{2s}\frac{(2s)!}{(s!)^2}\frac{B_{2\ell-2s}}{(2\ell-2s)}. \quad (35)$$

By equating (32) and (35), the terms logarithmically diverging for small $x$ cancel and we obtain the relation

$$\sum_{j=1}^{\ell}\left[S_{2j}^Y-\frac{2}{\pi}\cdot\frac{(-1)^j}{j}\right](-1)^{\ell-j}\frac{(k/2)^{2\ell}}{(\ell-j)!(\ell+j)!}-\frac{2}{d}\left\{\sum_{n\in\overline{\Omega}^+}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right]-\sum_{n\in\Omega^+}\frac{1}{\alpha_n}\right\}(-1)^\ell\frac{(k/2)^{2\ell}}{(\ell!)^2}$$
$$=-\frac{(-1)^\ell}{(2\ell)!}\frac{2}{d}\left\{\sum_{n\in\overline{\Omega}^+}\alpha_n^{2\ell}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right]-\sum_{n\in\Omega^+}\frac{\alpha_n^{2\ell}}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right\}$$
$$-\frac{1}{\pi}(-1)^\ell\frac{(k/2)^{2\ell}}{(\ell!)^2}\left(\sum_{p=1}^{2\ell}\frac{1}{p}\right)+\frac{1}{\pi}(-1)^\ell\frac{K^{2\ell}}{(2\ell)!}\sum_{s=0}^{\ell-1}\left(\frac{k}{2K}\right)^{2s}\frac{(2s)!}{(s!)^2}\frac{B_{2\ell-2s}}{(2\ell-2s)}. \quad (36)$$

This is a recurrence relation for the lattice sums. If we separate $S_{2\ell}^Y$, (36) becomes

$$(-1)^\ell S_{2\ell}^Y = \frac{2}{\pi\ell} - \sum_{j=1}^{\ell-1}\left\{\left[S_{2j}^Y - \frac{2}{\pi}\frac{(-1)^j}{j}\right](-1)^j\frac{(2\ell)!}{(\ell-j)!(\ell+j)!}\right\} + \frac{2}{d}\frac{(2\ell)!}{(\ell!)^2}\left\{\sum_{n\in\overline{\Omega}^+}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right] - \sum_{n\in\Omega^+}\frac{1}{\alpha_n}\right\}$$
$$-\frac{2}{d}\left(\frac{2}{k}\right)^{2\ell}\left\{\sum_{n\in\overline{\Omega}^+}\alpha_n^{2\ell}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right]\right.$$
$$\left. - \sum_{n\in\Omega^+}\alpha_n^{2\ell-1}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right\} - \frac{1}{\pi}\frac{(2\ell)!}{(\ell!)^2}\left(\sum_{p=1}^{2\ell}\frac{1}{p}\right) + \frac{1}{\pi}\sum_{s=0}^{\ell-1}\left(\frac{2K}{k}\right)^{2\ell-2s}\frac{(2s)!}{(s!)^2}\frac{B_{2\ell-2s}}{2\ell-2s}\ . \tag{37}$$

Taking into account the Taylor series of $1/|\chi_n|$, for $n\in\overline{\Omega}^+$, we have

$$\frac{2}{d}\left(\frac{2}{k}\right)^{2\ell}\sum_{n\in\overline{\Omega}^+}\alpha_n^{2\ell}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\sum_{s=0}^{\ell}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)\right] = \frac{2}{d}\left(\frac{2}{k}\right)^{2\ell}\sum_{n\in\overline{\Omega}^+}\alpha_n^{2\ell-1}\sum_{s=\ell+1}^{\infty}(-1)^s\left(\frac{k}{\alpha_n}\right)^{2s}P_{2s}(0)$$
$$= \frac{1}{\pi}\sum_{s=\ell+1}^{\infty}\frac{(2s)!}{(s!)^2}\left(\frac{2K}{k}\right)^{2\ell-2s}\sum_{n=m+1}^{\infty}\frac{1}{n^{2s-2\ell+1}}$$
$$= \frac{1}{\pi}\sum_{s=\ell+1}^{\infty}\frac{(2s)!}{(s!)^2}\left(\frac{2K}{k}\right)^{2\ell-2s}\zeta(2s-2\ell+1,m+1)\ , \tag{38}$$

where $2m\pi < kd < 2(m+1)\pi$ and $\zeta(s,m)$ is the generalized Riemann zeta function [18].

Finally, the recurrence relation for the lattice sums $S_{2\ell}^Y$, $\ell\geq 1$, may be written in the form

$$(-1)^\ell S_{2\ell}^Y = -\frac{1}{2}\frac{(2\ell)!}{(\ell!)^2}S_0^Y - \sum_{j=1}^{\ell-1}\left\{\left[S_{2j}^Y - \frac{2}{\pi}\frac{(-1)^j}{j}\right](-1)^j\frac{(2\ell)!}{(\ell-j)!(\ell+j)!}\right\}$$
$$+\frac{2}{\pi\,\ell} - \frac{1}{\pi}\frac{(2\ell)!}{(\ell!)^2}\left[\ln\left(\frac{k}{2K}\right)+\gamma\right] + \frac{1}{\pi}\sum_{s=0}^{\ell}\frac{(2s)!}{(s!)^2}\left(\frac{2K}{k}\right)^{2\ell-2s}\sum_{n\in\Omega^+}\frac{1}{n^{2s-2\ell+1}}$$
$$+\frac{1}{\pi}\sum_{s=0}^{\ell-1}\frac{(2s)!}{(s!)^2}\left(\frac{2K}{k}\right)^{2\ell-2s}\frac{B_{2\ell-2s}}{2\ell-2s} - \frac{1}{\pi}\frac{(2\ell)!}{(\ell!)^2}\left(\sum_{p=1}^{2\ell}\frac{1}{p}\right) - \frac{1}{\pi}\sum_{s=\ell+1}^{\infty}\frac{(2s)!}{(s!)^2}\left(\frac{2K}{k}\right)^{2\ell-2s}\zeta(2s-2\ell+1,m+1) \tag{39}$$

and $S_0^Y$ is given by (31).

This recurrence relation does not appear to have beeen derived previously. Examples of its application are

$$S_2^Y(k,d) = 2\sum_{n=1}^{\infty}Y_2(nkd)$$
$$= \frac{1}{\pi} - \frac{1}{\pi}\left(\frac{K}{k}\right)^2\left[\frac{1}{3}+2m(m+1)\right] - \frac{2}{\pi}\sum_{n=m+1}^{\infty}\left[\frac{1}{\sqrt{n^2-(k/K)^2}}-\frac{1}{n}\right]$$
$$+\frac{1}{\pi}\left(\frac{2K}{k}\right)^2\sum_{s=2}^{\infty}\frac{(2s)!}{(s!)^2}\left(\frac{k}{2K}\right)^{2s}\zeta(2s-1,m+1) \tag{40}$$

and

$$S_4^Y(k,d) = 2\sum_{n=1}^{\infty}Y_4(nkd)$$
$$= \frac{1}{2\pi} - \frac{2}{\pi}\left(\frac{K}{k}\right)^2\left[\frac{1}{3}+2m(m+1)\right] - \frac{2}{\pi}\left(\frac{K}{k}\right)^4\left[\frac{1}{15}-2m^2(m+1)^2\right]$$
$$+\frac{6}{\pi}\sum_{n=m+1}^{\infty}\left[\frac{1}{\sqrt{n^2-(k/K)^2}}-\frac{1}{n}\right] - \frac{1}{\pi}\left(\frac{2K}{k}\right)^4\sum_{s=3}^{\infty}\frac{(2s)!}{(s!)^2}\left(\frac{k}{2K}\right)^{2s}\zeta(2s-3,m+1),$$

where $m < k/K < m+1$ .

### B. Green's function in terms of lattice sums

In the case of normal incidence ($\alpha_0 = 0$), (2) takes the form

$$G_d(x,y) = \frac{1}{4i}\sum_{n\in\mathcal{Z}} H_0^{(1)}(k|\mathbf{r}-\mathbf{R_n}|) = \frac{1}{4i}\left[H_0^{(1)}(kr) + \sum_{n\in\mathcal{Z}^*} H_0^{(1)}(k|\mathbf{r}-\mathbf{R_n}|)\right], \tag{41}$$

where $\mathbf{r} = (x,y)$ and $\mathbf{R_n} = (nd,0)$. Within the unit cell $(-d/2 \le x \le d/2, -d/2 \le y \le d/2)$ we have $r < R_n$, $\forall n \neq 0$ and we apply the addition theorem for Bessel functions [12]. In this way (41) becomes

$$G_d(x,y) = \frac{1}{4i}\left[H_0^{(1)}(kr) + \sum_{\ell=-\infty}^{\infty} S_\ell(k,d)J_\ell(kr)\, e^{-i\ell\theta}\right], \tag{42}$$

where the lattice sums $S_\ell$ are defined in (20) and $\theta = \arctan(y/x)$. Only the lattice sums of even order are different from zero such that (42) may be written as

$$G_d(x,y) = \frac{1}{4i}\left[H_0^{(1)}(kr) + S_0(k,d)J_0(kr) + \sum_{\ell\in\mathcal{Z}^*} S_{2\ell}(k,d)J_{2\ell}(kr)\, e^{-2i\ell\theta}\right] = \frac{1}{4i}\left[H_0^{(1)}(kr) + S_0(k,d)J_0(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}(k,d)J_{2\ell}(kr)\, \cos(2\ell\theta)\right]. \tag{43}$$

In this way the Green's function (2) is represented as a Neumann series with coefficients given by the lattice sums. Physical arguments indicate that the radius of convergence of the series in (43) is $r = d$. [These physical arguments are based on the location of sources of the periodic Green's function, which are at $x = 0$ —represented by $H_0^{(1)}(kr)$ in (43)—and $x = nd$ ($n = \pm1, \pm2, \ldots$)—represented by the series in (43). They are supported, mathematically, by the asymptotic estimates for the $S_{2\ell}$ with $\ell$ large, discussed below.]

### C. First-order derivatives of the Green's function

The first order derivatives of Green's function (43) are given by the formulas:

$$\frac{\partial G_d}{\partial x} = \frac{1}{4i}\left\{\left[H_0^{(1)'}(kr) + S_0(k,d)J_0'(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}(k,d)J_{2\ell}'(kr)\, \cos(2\ell\theta)\right]\frac{kx}{r} - 4\sum_{\ell=1}^{\infty} \ell S_{2\ell}(k,d)J_{2\ell}(kr)\, \sin(2\ell\theta)\frac{\partial\theta}{\partial x}\right\}, \tag{44}$$

$$\frac{\partial G_d}{\partial y} = \frac{1}{4i}\left\{\left[H_0^{(1)'}(kr) + S_0(k,d)J_0'(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}(k,d)J_{2\ell}'(kr)\, \cos(2\ell\theta)\right]\frac{ky}{r} - 4\sum_{\ell=1}^{\infty} \ell S_{2\ell}(k,d)J_{2\ell}(kr)\, \sin(2\ell\theta)\frac{\partial\theta}{\partial y}\right\}, \tag{45}$$

for $y \ge 0$. Here, $\partial\theta/\partial x = -y/r^2$ and $\partial\theta/\partial y = x/r^2$.

Substituting the derivatives of the Bessel functions:

$$J_{2\ell}'(z) = -J_{2\ell+1}(z) + \frac{2\ell}{z}J_{2\ell}(z),$$
$$H_0^{(1)'}(z) = -H_1^{(1)}(z),$$

we obtain

$$\frac{\partial G_d}{\partial x} = \frac{1}{4i}\left\{\left[H_1^{(1)}(kr) + S_0(k,d)J_1(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}(k,d)J_{2\ell+1}(kr)\, \cos(2\ell\theta)\right]\left(-\frac{kx}{r}\right) + \frac{4}{r^2}\sum_{\ell=1}^{\infty} S_{2\ell}(k,d)J_{2\ell}(kr)\, \ell\, [x\cos(2\ell\theta) + y\sin(2\ell\theta)]\right\}, \tag{46}$$

$$\frac{\partial G_d}{\partial y} = \frac{1}{4i}\left\{\left[H_1^{(1)}(kr) + S_0(k,d)J_1(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}(k,d)J_{2\ell+1}(kr)\, \cos(2\ell\theta)\right]\left(-\frac{ky}{r}\right) + \frac{4}{r^2}\sum_{\ell=1}^{\infty} S_{2\ell}(k,d)J_{2\ell}(kr)\, \ell\, [-x\sin(2\ell\theta) + y\cos(2\ell\theta)]\right\}, \tag{47}$$

for $y \ge 0$.

## IV. NUMERICAL RESULTS

The main advantage of using the lattice sums method is that, for a given set $(k,d)$, the coefficients of the se-

TABLE I. Normal incidence. The first 22 values of $S^J_{2\ell}$ and $S^Y_{2\ell}$ for $\lambda < d$ and $\lambda > d$ ($d = 1$), together with the nearest-neighbor estimates $S^Y_{2\ell} \approx 2\,Y_{2\ell}(kd)$.

| | $\lambda = 0.23$ | | | $\lambda = 1.77$ | | |
|---|---|---|---|---|---|---|
| $2\ell$ | $S^J_{2\ell}$ | $S^Y_{2\ell}$ | $2\,Y_{2\ell}(kd)$ | $S^J_{2\ell}$ | $S^Y_{2\ell}$ | $2\,Y_{2\ell}(kd)$ |
| 0 | −0.035528 | 0.199540 | 0.300607 | −0.43659 | 0.28088 | 0.33701 |
| 2 | 0.053703 | −0.198820 | −0.304103 | 0.56341 | 0.07074 | 0.12868 |
| 4 | −0.108150 | 0.187800 | 0.304812 | 0.56341 | −0.92948 | −1.28066 |
| 6 | 0.191780 | −0.140160 | −0.273319 | 0.56341 | −5.04250 | −4.92973 |
| 8 | −0.270990 | 0.020452 | 0.167699 | 0.56341 | $-5.3040 \times 10^{1}$ | $-5.2099 \times 10^{1}$ |
| 10 | 0.266130 | 0.181310 | 0.032814 | 0.56341 | $-1.0691 \times 10^{3}$ | $-1.0653 \times 10^{3}$ |
| 12 | −0.076179 | −0.380830 | −0.258540 | 0.56341 | $-3.4789 \times 10^{4}$ | $-3.4766 \times 10^{4}$ |
| 14 | −0.290020 | 0.364100 | 0.309130 | 0.56341 | $-1.6447 \times 10^{6}$ | $-1.6445 \times 10^{6}$ |
| 16 | 0.536910 | 0.035812 | −0.019554 | 0.56341 | $-1.0604 \times 10^{8}$ | $-1.0604 \times 10^{8}$ |
| 18 | −0.244020 | −0.520380 | −0.337140 | 0.56341 | $-8.9274 \times 10^{9}$ | $-8.9274 \times 10^{9}$ |
| 20 | −0.354790 | 0.384150 | 0.117792 | 0.56341 | $-9.5014 \times 10^{11}$ | $-9.5014 \times 10^{11}$ |
| 22 | 0.268740 | 0.167120 | 0.389813 | 0.56341 | $-1.2466 \times 10^{14}$ | $-1.2466 \times 10^{14}$ |
| 24 | 0.069628 | 0.122980 | 0.111452 | 0.56341 | $-1.9761 \times 10^{16}$ | $-1.9761 \times 10^{16}$ |
| 26 | 0.687400 | −0.014258 | −0.297882 | 0.56341 | $-3.7222 \times 10^{18}$ | $-3.7223 \times 10^{18}$ |
| 28 | 0.277790 | −1.061700 | −0.621598 | 0.56341 | $-8.2168 \times 10^{20}$ | $-8.2168 \times 10^{20}$ |
| 30 | −0.306420 | −0.841700 | −1.096150 | 0.56341 | $-2.1008 \times 10^{23}$ | $-2.1008 \times 10^{23}$ |
| 32 | 0.484990 | −2.346700 | −2.531620 | 0.56341 | $-6.1583 \times 10^{25}$ | $-6.1583 \times 10^{25}$ |
| 34 | −0.087253 | −8.393500 | −7.935630 | 0.56341 | $-2.0516 \times 10^{28}$ | $-2.0516 \times 10^{28}$ |
| 36 | −0.274410 | −31.299000 | −31.578300 | 0.56341 | $-7.7072 \times 10^{30}$ | $-7.7072 \times 10^{30}$ |
| 38 | 0.261040 | −152.080000 | −152.099000 | 0.56341 | $-3.2429 \times 10^{33}$ | $-3.2429 \times 10^{33}$ |
| 40 | −0.144210 | −862.520000 | −862.473000 | 0.56341 | $-1.5189 \times 10^{36}$ | $-1.5189 \times 10^{36}$ |
| 42 | 0.290140 | −5652.200000 | −5652.260000 | 0.56341 | $-7.8758 \times 10^{38}$ | $-7.8758 \times 10^{38}$ |

ries (43,46,47) have to be evaluated once only. This increases appreciably the speed of numerical evaluation of the Green's function and its derivatives at any point in the $xy$ plane.

For numerical calculations, the series contained in (31) converges slowly. The convergence can be accelerated by means of Kummer's method. We start with the series

$$\sum_{n=m+1}^{\infty}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right] = \sum_{n=m+1}^{\infty}\frac{1}{nK}\left[\frac{1}{\sqrt{1-(k/(nK))^2}}-1\right], \quad (48)$$

TABLE II. Normal incidence. Comparison between different numerical methods to evaluate the Green's function ($d = 1$). The columns 5 and 6 display the real and imaginary parts of the Green's function, $N$ represents the number of terms in the corresponding series and $T_n$ is the CPU time, in seconds, required for $n$ independent evaluations.

| Eq. | $\lambda$ | $x$ | $y$ | $\mathrm{Re}[G(x,y)]$ | $\mathrm{Im}[G(x,y)]$ | $N$ | $T_1$ | $T_{50}$ | $T_{100}$ |
|---|---|---|---|---|---|---|---|---|---|
| (5) | 0.23 | 0.2 | 0.03 | -0.0501668250134190 | 0.0108324843142530 | 159 | 3 | 154 | 343 |
| (11) | | | | -0.0501668250134191 | 0.0108324843142530 | 121 | 6 | 299 | 629 |
| (43) | | | | -0.0501668250137788 | 0.0108324843138182 | 11 | 37 | 73 | 111 |
| (43) | | | | -0.0501668250134200 | 0.0108324843142531 | 21 | 81 | 231 | 388 |
| (5) | 0.23 | 0.2 | 0.003 | -0.0502817699735941 | 0.0154319789780036 | 1449 | 27 | 1443 | 3072 |
| (11) | | | | -0.0502817699735942 | 0.0154319789780036 | 876 | 38 | 1940 | 4131 |
| (43) | | | | -0.0502817699733261 | 0.0154319789783318 | 11 | 37 | 74 | 109 |
| (43) | | | | -0.0502817699735968 | 0.0154319789780035 | 21 | 81 | 229 | 386 |
| (5) | 0.23 | 0.2 | 0.0003 | -0.0502814167514775 | 0.0154784735299674 | 13294 | 318 | 13184 | 26292 |
| (11) | | | | -0.0502814167514774 | 0.0154784735299674 | 5746 | 246 | 12023 | 25691 |
| (43) | | | | -0.0502814167511948 | 0.0154784735303132 | 11 | 36 | 73 | 103 |
| (43) | | | | -0.0502814167514801 | 0.0154784735299671 | 21 | 81 | 228 | 362 |

where $m < k/K < m+1$. The general term has the asymptotic expansion

$$\frac{1}{nK}\left[\frac{1}{\sqrt{1-(k/(nK))^2}}-1\right] = \frac{1}{nK}\sum_{j=1}^{\infty}(-1)^j\left(\frac{k}{nK}\right)^{2j}P_{2j}(0) \approx -\frac{k^2}{(nK)^3}P_2(0)+\frac{k^4}{(nK)^5}P_4(0), \quad (49)$$

and the asymptotic series corresponding to (48) has the closed-form sum

$$\frac{1}{2}P_2(0)\frac{k^2}{K^3}\psi^{(2)}(m+1)-\frac{1}{24}P_4(0)\frac{k^4}{K^5}\psi^{(4)}(m+1). \quad (50)$$

Here, $\psi^{(n)}(z)$ is the polygamma function [18]. By means of (49) and (50) the series (48) may be replaced by the series

$$\sum_{n=m+1}^{\infty}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}\right] = \sum_{n=m+1}^{\infty}\left[\frac{1}{|\chi_n|}-\frac{1}{\alpha_n}+\frac{k^2}{\alpha_n^3}P_2(0)-\frac{k^4}{\alpha_n^5}P_4(0)\right] +\frac{1}{2}P_2(0)\frac{k^2}{K^3}\psi^{(2)}(m+1) -\frac{1}{24}P_4(0)\frac{k^4}{K^5}\psi^{(4)}(m+1), \quad (51)$$

converging as $O(1/n^6)$.

The numerical values in Tables I and II were obtained with a *Mathematica* program run on a SPARC-10 workstation.

Table I displays the values of the first 22 lattice sums in two particular cases for $\lambda > d$ and $\lambda < d$. Note the behavior of the lattice sums $S_{2\ell}^Y$. Their magnitudes are small until their order $(2\ell)$ becomes comparable with $kd$, at which point they increase rapidly. In this region of large magnitudes, the $S_{2\ell}^Y$ are well approximated by the nearest-neighbors estimate

$$S_{2\ell}^Y(k,d) \approx 2Y_{2\ell}(kd). \quad (52)$$

For the same values of $\lambda$ and $d$ we give in Figs. 1 and 2 two examples of partial sums:

$$S_{2\ell}^{J(n)}(k,d) = 2\sum_{m=1}^{n} J_{2\ell}(mkd)\ , \quad (53)$$

$$S_{2\ell}^{Y(n)}(k,d) = 2\sum_{m=1}^{n} Y_{2\ell}(mkd)\ , \quad (54)$$

as functions of $n$. The dashed lines represent the values given by (25) and (39). Note that a prohibitive large number of terms would be required to evaluate these series to high accuracy by direct summation.

In Table II, the timing $(T_1)$ for Eq.(43) represents the time required to evaluate the Green's function for the first point $(x,y)$. To do this, a set of lattice sums $S_{2n}$

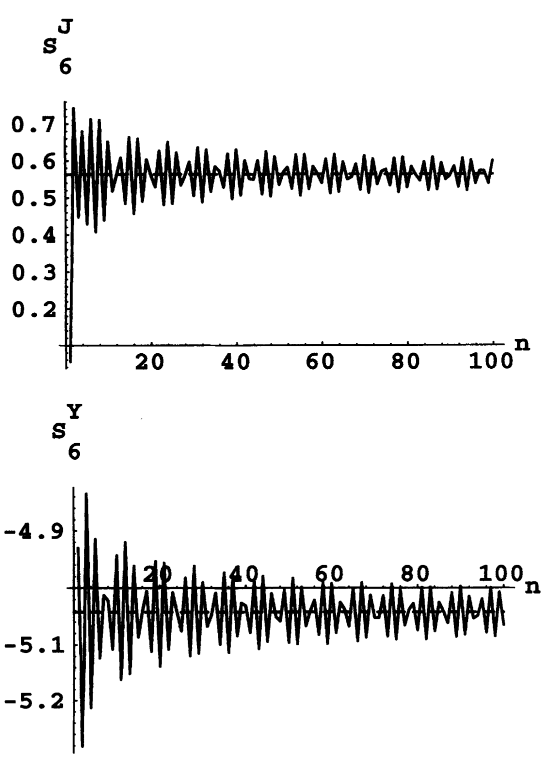


FIG. 1. The lattice sums $S_6^J$ and $S_6^Y$ as functions of the number of terms considered in the corresponding series, for $\lambda = 1.77$, $d = 1$. The dashed lines represent the values given by (25) and (39), respectively.

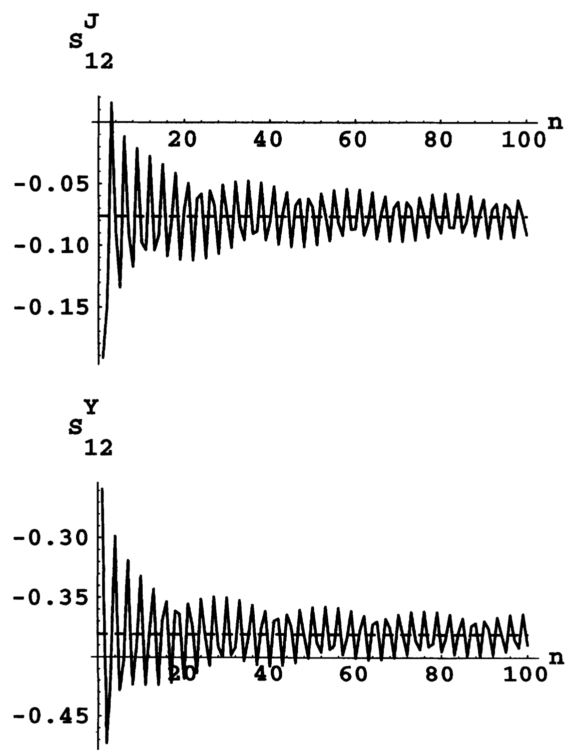


FIG. 2. The lattice sums $S_{12}^J$ and $S_{12}^Y$ as functions of the number of terms considered in the corresponding series, for $\lambda = 0.23$, $d = 1$. The dashed lines represent the values given by (25) and (39), respectively.

up to order $n = N - 1$ has to be evaluated. All other subsequent evaluations of the Green's function, at any other point $(x, y)$, use this set, and so require far less computation time. As can be seen from Table II, the use of Eq. (5) for $|y| > 0.03$ is computationally advantageous, whereas for $|y| < 0.03$, Eq. (43) is superior if more than three Green's function evaluations are required. If only the Green's function, and not its derivatives are required, the use of the third-order formulas is not computationally advantageous, compared with direct summation of (5), unless $y$ is very small ($|y| \leq 0.0003$ for the data here).

In (5) and (11) we stopped the series when the relative difference of two successive partial sums was less than $10^{-15}$. From (43) we obtain the same numerical value, with a high accuracy, summing only a reduced number of terms.

In Figs. 3 and 4 we plot the real and imaginary parts of $G(x, y)$ for a short wavelength, for two values of $y$. Note the development of the logarithmic singularity in the real part of $G(x, y)$ as $x$ tends to zero [see Eq. (42)]. This singularity is pronounced for $|y|$ small (Fig. 4) but is much less evident when $|y|$ is increased (Fig. 3). For a longer wavelength, we see from Figs. 5 and 6 that the imaginary part of $G(x, y)$ is effectively constant, while the contribution of the logarithmic term to the real part has become the dominant feature, with the oscillations evident in Figs. 3 and 4 having disappeared.

In Figs. 7 and 8 we display the behavior of $G(x, y)$ as a function of $x$ for an off-axis case ($\theta_i = \pi/6$). Once again,

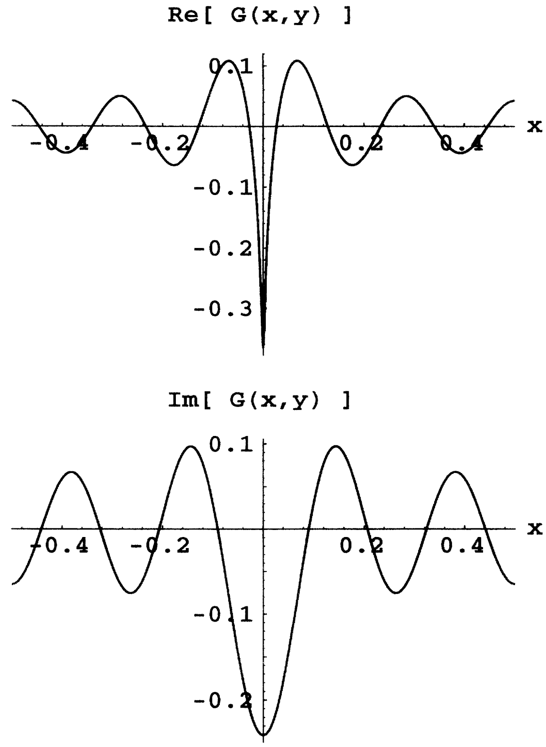


FIG. 4. Normal incidence. The real and imaginary parts of the Green's function $G(x, y)$ for $y = 0.003$ and $\lambda = 0.23$ ($d = 1$).

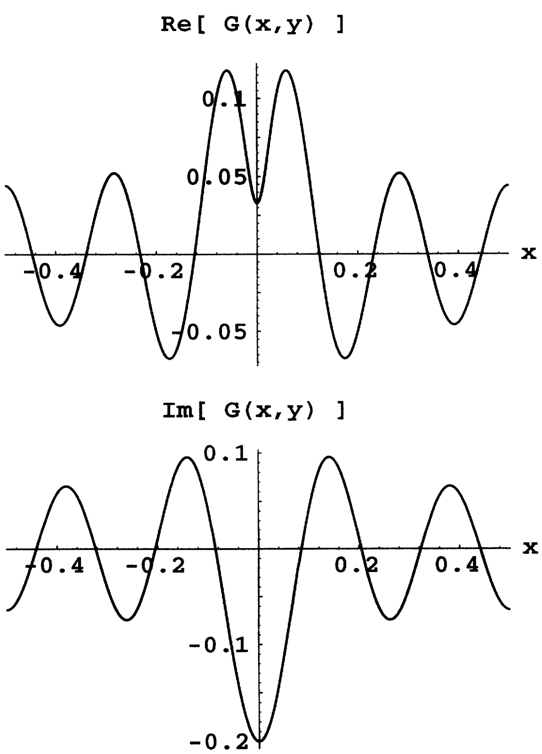


FIG. 3. Normal incidence. The real and imaginary parts of the Green's function $G(x, y)$ for $y = 0.03$ and $\lambda = 0.23$ ($d = 1$).

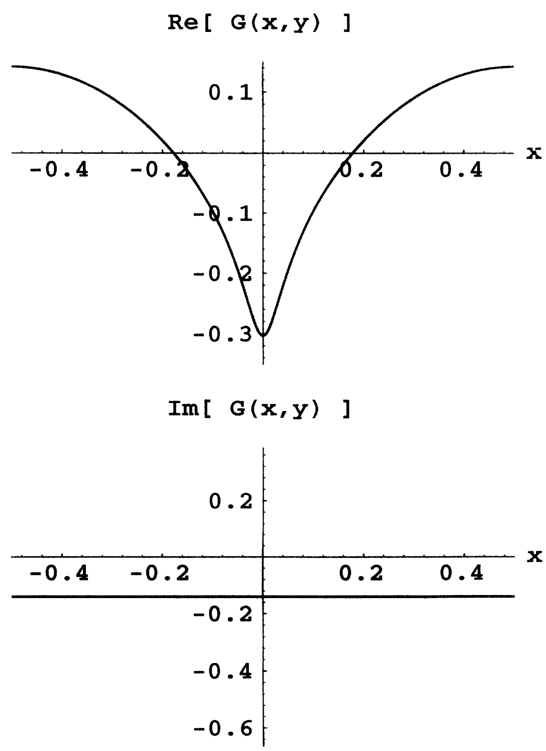


FIG. 5. Normal incidence. The real and imaginary parts of the Green's function $G(x, y)$ for $y = 0.03$ and $\lambda = 1.77$ ($d = 1$).

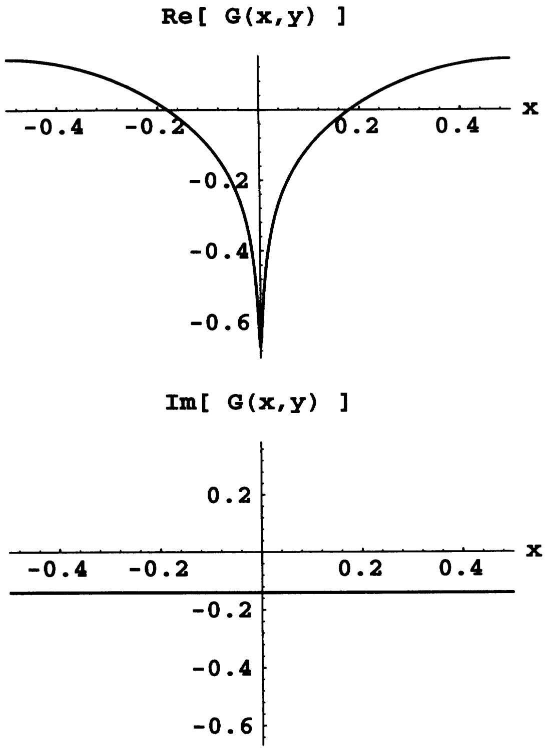


FIG. 6. Normal incidence. The real and imaginary parts of the Green's function $G(x,y)$ for $y = 0.003$ and $\lambda = 1.77$ ($d = 1$).

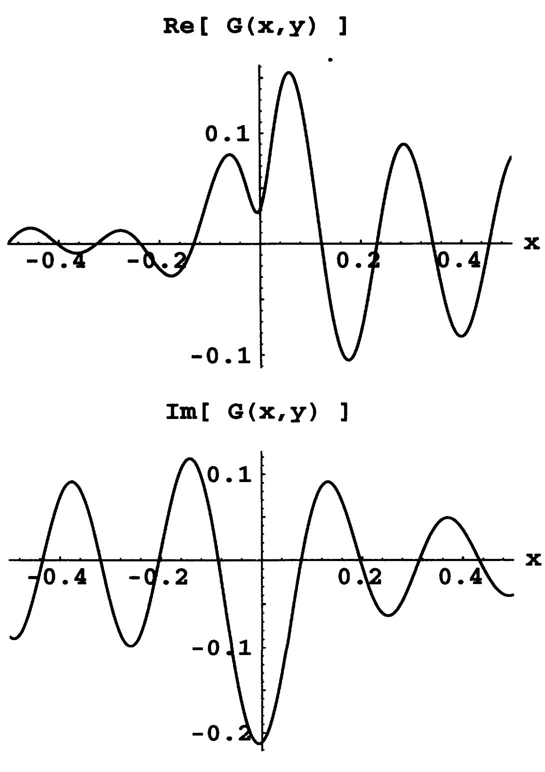


FIG. 7. Off-axis incidence. The real and imaginary parts of the Green's function $G(x,y)$ for $y = 0.03$, $\theta_i = \pi/6$, and $\lambda = 0.23$ ($d = 1$).

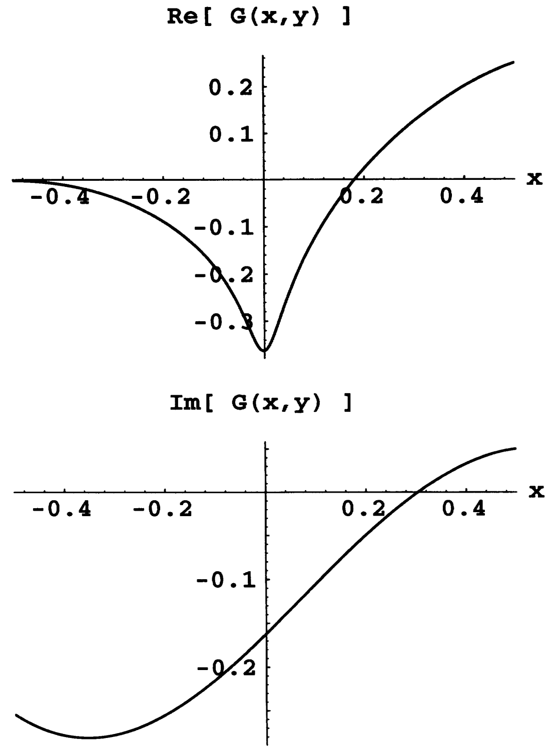


FIG. 8. Off-axis incidence. The real and imaginary parts of the Green's function $G(x,y)$ for $y = 0.03$, $\theta_i = \pi/6$, and $\lambda = 1.77$ ($d = 1$).

at a short wavelength both the real and imaginary parts of $G(x,y)$ exhibit oscillations. At a longer wavelength, these oscillations are gone, but the effect of the nonzero angle of incidence is clear: the imaginary part of $G$ now varies with $x$, as the phase factor $\exp(i\alpha_0 x)$ effectively "mixes" the real and imaginary parts.

## V. CONCLUSIONS

We have considered spectral and spatial expansions for the Green's function for grating diffraction problems. For the former, we have exhibited cubically convergent expansions for the Green's function, and its $x$ and $y$ derivatives. These cubically convergent expansions are preferable to direct summation for the Green's function only for points very close to the grating plane (i.e., for small values of $y$). If spatial derivatives of the Green's function are required, then direct summation becomes less attractive by comparison with the (somewhat more complicated) cubically convergent expansions.

The spatial expansions seem to us to provide the method of choice for evaluating the Green's function and its spatial derivatives, if accurate values at a number of points with $|y|$ small are required. The prerequisite for efficient use of spatial expansion is the accurate evaluation of lattice sums, and we have given a method for the evaluation of lattice sums for normally incident radiation. We are currently attempting to find methods for evaluating lattice sums for off-axis incidence. Our investigations of this question have revealed that the techniques outlined in this paper remain valid in principle. However, numerical difficulties, associated with ill-conditioned expressions for lattice sums of high order, require adaptations of the methods which are still under investigation.

## ACKNOWLEDGMENTS

This work was undertaken while one of the authors (N. A. Nicorovici) was the recipient of an Australian Research Council large grant. R. Petit acknowledges support from the Australian Research Council through a small grant which made possible his participation in this work. The support of the Science Foundation for Physics within the University of Sydney is also acknowledged.

## APPENDIX: FORMULAS FOR COMPUTATION OF TRANSCENDENTAL FUNCTIONS

The series expansion of the polylogarithm function may be obtained starting with the expansion [19]

$$\frac{z}{e^z-1} = 1 - \frac{z}{2} + \sum_{n=2}^{\infty} B_n \frac{z^n}{n!},$$

where $B_n$ are the Bernoulli numbers. Dividing by $z$ and integrating over $z$ from 0 to $z$, we obtain

$$\ln(1-e^{-z}) = \ln z - \frac{z}{2} + \sum_{n=2}^{\infty} B_n \frac{z^n}{n!\,n} ,$$

which gives the series expansion of the function [19]:

$$\mathrm{Li}_1(e^{-z}) \stackrel{\text{def}}{=} \sum_{n=1}^{\infty} \frac{e^{-nz}}{n} = -\ln(1-e^{-z}) . \qquad \text{(A1)}$$

The polylogarithm function $\mathrm{Li}_s(z)$ is related to the Lerch phi function $\Phi(z,s,v)$ [18], and has the series expansion:

$$\begin{aligned}\mathrm{Li}_s(z) &\stackrel{\text{def}}{=} \sum_{n=1}^{\infty} \frac{z^n}{n^s} = z\,\Phi(z,s,1) \\ &= \sum_{n=0}^{\infty}{}' \zeta(s-n)\frac{(\ln z)^n}{n!} \\ &\quad + \frac{(\ln z)^{s-1}}{(s-1)!}\left[\psi(s)-\psi(1)-\ln(\ln 1/z)\right] . \qquad \text{(A2)}\end{aligned}$$

Here, the prime indicates that the term with $n = s-1$ is to be omitted. Also, $\zeta(s)$ is the Riemann zeta function [18] and $\psi(s)$ is the digamma function [18] [$\psi(1) = -\gamma = -0.577\,216$]. The series expansion (A2) is valid for $s = 2,3,4,\ldots$ and $|\ln z| < 2\pi$.

The derivatives of the polylogarithm function are given by the expressions

$$\frac{d}{dz}\mathrm{Li}_2(z) = -\frac{1}{z}\ln(1-z), \qquad \text{(A3)}$$

$$\frac{d}{dz}\mathrm{Li}_s(z) = \frac{1}{z}\mathrm{Li}_{s-1}(z)\,,\ s = 3,4,\ldots . \qquad \text{(A4)}$$

In all these expressions, we see there exists a logarithmic term. This implies a branch cut, which for $\Phi(z,s,v)$ and $\mathrm{Li}_s(z)$ is taken to run from $z = 1$ along the positive real axis. $\Phi$ and $\mathrm{Li}_s$ are then analytic in the cut plane [18].

In particular, if $z \to e^z$, the expansion (A2) becomes

$$\begin{aligned}\mathrm{Li}_s(e^z) &= \sum_{n=0}^{\infty}{}' \zeta(s-n)\frac{z^n}{n!} + \frac{z^{s-1}}{(s-1)!}\left[\psi(s)+\gamma-\ln(-z)\right] \\ &= \sum_{n=0}^{s-2} \zeta(s-n)\frac{z^n}{n!} + \frac{z^{s-1}}{(s-1)!}\left[\psi(s)+\gamma-\ln(-z)\right] \\ &\quad + B_1\frac{z^s}{s!} - \sum_{n=s+1}^{\infty} \frac{B_{n-s+1}}{n-s+1}\frac{z^n}{n!} , \qquad \text{(A5)}\end{aligned}$$

valid for $s \geq 2$ and $|z| < 2\pi$. To obtain (A5) we have used the relation between the Riemann zeta function and Bernoulli numbers: $\zeta(-n) = -B_{n+1}/(n+1)$, $\zeta(0) = B_1$. Also, $\psi(s) + \gamma = \sum_{p=1}^{s-1} 1/p$.

For numerical evaluations of $\mathrm{Li}_s(e^z)$, if $|z| < 1$, we need $\sim 6$ nonzero terms in the series to obtain an accuracy of $10^{-12}$. We mention that in (10) and (13), we have $z = -K|y| + iKx$, so that $|z| = Kr = 2\pi r/d$. Consequently, the convergence radius for (A5) is $r < d$; i.e., the expansion (A5) is valid at any point within the unit cell ($r \leq d/\sqrt{2}$).

From (A1), with $z = -i\theta$, we obtain the Clausen function $\mathrm{Cl}_1$:

$$\begin{aligned}\mathrm{Cl}_1(\theta) &\stackrel{\text{def}}{=} \mathrm{Re}\left[\mathrm{Li}_1(e^{i\theta})\right] = \sum_{n=1}^{\infty}\frac{\cos(n\theta)}{n} \\ &= -\ln|\theta| - \sum_{n=1}^{\infty} B_{2n}(-1)^n \frac{\theta^{2n}}{(2n)!(2n)},\end{aligned}$$

for $0 < \theta < 2\pi$. The generalized Clausen function is defined as [19]

$$\mathrm{Cl}_{2s+1}(\theta) = \sum_{n=1}^{\infty}\frac{\cos(n\theta)}{n^{2s+1}} = \mathrm{Re}\left[\mathrm{Li}_{2s+1}(e^{i\theta})\right] ,$$

$$\mathrm{Cl}_{2s+2}(\theta) = \sum_{n=1}^{\infty}\frac{\sin(n\theta)}{n^{2s+2}} = \mathrm{Im}\left[\mathrm{Li}_{2s+2}(e^{i\theta})\right] ,$$

for $s = 0,1,2,\ldots$ and, from the series expansion (A5), we obtain

$$\begin{aligned}\mathrm{Cl}_{2s+1}(\theta) &= \sum_{n=0}^{s-1}\frac{\zeta(2s+1-2n)}{(2n)!}(-1)^n\theta^{2n} \\ &\quad + \frac{(-1)^s}{(2s)!}\left(\sum_{p=1}^{2s}\frac{1}{p}\right)\theta^{2s} - (-1)^s\frac{\theta^{2s}}{(2s)!}\ln|\theta| \\ &\quad - (-1)^s\sum_{n=1}^{\infty} B_{2n}(-1)^n\frac{\theta^{2n+2s}}{(2n+2s)!(2n)} . \qquad \text{(A6)}\end{aligned}$$

This series expansion is valid for $0 < \theta < 2\pi$. We mention that, in (33), $0 < x < d$ and, therefore, $0 < Kx < 2\pi$.

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