Lattice sums for off-axis 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 at a general angle in the xy plane on a singly periodic structure, or grating, oriented along the x axis. We equate the spatial and spectral forms of the Green's function, and so establish expressions from which grating lattice sums can be evaluated for oblique incidence. We also obtain a set of identities among the lattice sums. We use these lattice sums in an expression for the Green's function, which we show to be computationally fast, 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. 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 [1–5].

The spatial form represents the Green's function as 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 dependences. The spectral form represents the Green's function as a sum of plane waves, each obeying the appropriate quasiperiodicity condition [6]. 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 a previous paper [7], we have studied the case of normal incidence on a grating. We showed that the spatial form of the Green's function could be reexpressed in terms of lattice sums, giving a computationally efficient expression (provided numerical values of the Green's function were required at more than a few spatial points). Here, we consider the lattice sums and the expression for the Green's function, in the case of arbitrary incidence and quasiperiodicity. We equate the spectral and spatial forms of the Green's function, expand the resultant identity using Graf's addition theorem, and solve for lattice sums. These lattice sums have only been evaluated hitherto for the zeroth order case [8]; here, we exhibit a recurrence formula which extends their calculation to higher orders. As this recurrence formula becomes unstable, numerically, for lattice sums of large orders, we derive a set of lattice sum identities. A hybrid technique, based on the recurrence formula and the lattice sum identities, combined with a simple asymptotic expression, is capable of providing accurate values (eight figures) of lattice sums of arbitrarily high order. We use the lattice sums to construct an 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 has to be evaluated at more than a few points. (The lattice sums are independent of the point at which the field is evaluated, and therefore the time penalty in calculating them is amortised over the number of Green function evaluations.) We also study the symmetry properties of the Green's function, related to the incidence angle and the reflection of axes.

We present numerical results confirming our method in both graphical and tabular form, in order to aid those wishing to implement our methods.

The methods we will describe refer to the spatial form of the Green's function expressed in terms of Hankel functions. The basis of Hankel functions does give rise to a complete expansion of diffracted fields, and is particularly well adapted to the discussion of gratings composed of wires, having a circular cross section. Our methods could be generalized to other bases of functions—for example, Weber functions (parabolic wires) or Mathieu functions (elliptical wires) [9].

II. LATTICE SUMS

The Green's function for a one-dimensional array of line sources spaced d units apart along the x axis, obeys the inhomogeneous Helmholtz equation:

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

and is given by

$$G(x,y;\alpha_0) = \frac{1}{4i} \sum_{n=-\infty}^{\infty} H_0^{(1)}(k\sqrt{(x-nd)^2 + y^2})\, e^{i\alpha_0 nd}, \quad (2)$$

where $H_0^{(1)}$ is the zeroth-order Hankel function of the first kind and k is the wave number of the medium. An alternative to evaluating the series in (2) is to evaluate the spectral domain Green's function [6]

$$G(x,y;\alpha_0) = \frac{1}{2id}\sum_{n=-\infty}^{\infty}\frac{1}{\chi_n}\,e^{i[\alpha_n x+\chi_n|y|]}, \tag{3}$$

where

$$\alpha_n = \alpha_0 + nK = \alpha_0 + \frac{2\pi n}{d},$$

$$\chi_n = \begin{cases}\sqrt{k^2-\alpha_n{}^2}\ , & \alpha_n^2 \le k^2\\ i\sqrt{\alpha_n{}^2-k^2}\ , & \alpha_n^2 > k^2\ .\end{cases} \tag{4}$$

A. Recurrence relation for lattice sums

By equating (2) and (3) we have

$$\sum_{n=-\infty}^{\infty} H_0^{(1)}\left(k\left|\sqrt{(x-nd)^2+y^2}\right|\right)e^{i\alpha_0 nd} = \frac{2}{d}\sum_{n=-\infty}^{\infty}\frac{1}{\chi_n}\,e^{i(\alpha_n x+\chi_n|y|)}\ . \tag{5}$$

We mention that this equation is invariant with respect to the translations $x \to x+md$, $\forall m \in \mathcal{Z}$.

Now, we assume that $y=0$ and $-d<x<d$, so that $|nd|>|x|$, $\forall n \neq 0$. In this case, (5) becomes

$$H_0^{(1)}(k|x|)+\sum_{n\neq 0}\sum_{\ell=-\infty}^{\infty} H_\ell^{(1)}(|n|kd)e^{i\ell\varphi_n}e^{i\alpha_0 nd} \times J_\ell(k|x|)e^{-i\ell\theta_x} = \frac{2}{d}\,e^{i\alpha_0 x}\sum_{n=-\infty}^{\infty}\frac{1}{\chi_n}\,e^{inKx}\ . \tag{6}$$

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

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

For oblique incidence ($\alpha_0 \neq 0$), the lattice sums are defined by the formula:

$$S_\ell(\alpha_0,k,d) = \sum_{n\neq 0} H_\ell^{(1)}(|n|kd)\ e^{i\alpha_0 nd}\ e^{i\ell\varphi_n}\ . \tag{7}$$

For brevity of notation, in what follows we will specify the arguments of the lattice sums S_ℓ only when necessary to avoid confusion. Starting with the definition (7), we have

$$\begin{aligned} S_\ell &= \sum_{n=1}^{\infty} H_\ell^{(1)}(nkd)e^{i\alpha_0 nd} + \sum_{n=-\infty}^{-1} H_\ell^{(1)}(|n|kd)e^{i\alpha_0 nd}e^{i\ell\pi}\\ &= \sum_{n=1}^{\infty} H_\ell^{(1)}(nkd)e^{i\alpha_0 nd} + \sum_{n=1}^{\infty}(-1)^\ell H_\ell^{(1)}(nkd)e^{-i\alpha_0 nd}\\ &= \sum_{n=1}^{\infty} H_\ell^{(1)}(nkd)\left[e^{i\alpha_0 nd}+(-1)^\ell e^{-i\alpha_0 nd}\right]\\ &= \sum_{n=1}^{\infty} H_\ell^{(1)}(nkd)\left\{\left[1+(-1)^\ell\right]\cos(\alpha_0 nd) + i\left[1-(-1)^\ell\right]\sin(\alpha_0 nd)\right\}\ . \end{aligned} \tag{8}$$

From the last formula we deduce the relation $S_{-\ell} = (-1)^\ell S_\ell$.

The real and imaginary parts of S_ℓ are given by the expressions

$$S_{2\ell} = 2\sum_{n=1}^{\infty} H_{2\ell}^{(1)}(nkd)\cos(\alpha_0 nd) \equiv S_{2\ell}^J + iS_{2\ell}^Y\ , \tag{9}$$

$$S_{2\ell+1} = 2i\sum_{n=1}^{\infty} H_{2\ell+1}^{(1)}(nkd)\sin(\alpha_0 nd) \equiv iS_{2\ell+1}^J - S_{2\ell+1}^Y\ , \tag{10}$$

where S^J and S^Y are the series involving the J and Y Bessel functions, respectively.

We also remark that the lattice sums satisfy the relation

$$S_{-\ell}J_{-\ell}(kx) = S_\ell J_\ell(kx)\ ,$$

so that, with x restricted to the range $0<x<d$, (6) may be written in the form

$$H_0^{(1)}(kx) + S_0J_0(kx) + 2\sum_{\ell=1}^{\infty} S_\ell J_\ell(kx) = \frac{2}{d}\,e^{i\alpha_0 x}\sum_{n=-\infty}^{\infty}\frac{1}{\chi_n}\,e^{inKx}\ . \tag{11}$$

Taking into account that $\alpha_0 = k \sin\theta_i$, θ_i being the incidence angle, and, consequently $k > |\alpha_0| \geq 0$, the right hand side of (11) may be separated into propagating and evanescent sums as follows:

$$\frac{2}{d}e^{i\alpha_0 x}\left[\frac{1}{\chi_0}+\sum_{n=1}^{n_1}\frac{e^{inKx}}{\sqrt{k^2-\alpha_n^2}}+\sum_{n=1}^{n_2}\frac{e^{-inKx}}{\sqrt{k^2-\alpha_{-n}^2}} + \sum_{n=n_1+1}^{\infty}\frac{e^{inKx}}{i\sqrt{\alpha_n^2-k^2}}+\sum_{n=n_2+1}^{\infty}\frac{e^{-inKx}}{i\sqrt{\alpha_{-n}^2-k^2}}\right],$$

where

$$2\pi n_1 < (k-\alpha_0)d < 2\pi(n_1+1)\ ,$$

$$2\pi n_2 < (k+\alpha_0)d < 2\pi(n_2+1)\ .$$

The separation of real and imaginary parts in (11) leads us to a pair of equations for the lattice sums:

$$(S_0^J+1)J_0(kx)+2\sum_{\ell=1}^{\infty}S_{2\ell}^J J_{2\ell}(kx)-2\sum_{\ell=0}^{\infty}S_{2\ell+1}^Y J_{2\ell+1}(kx)=\frac{2}{d}\left\{\frac{\cos(\alpha_0 x)}{\chi_0}+\sum_{n=1}^{n_1}\frac{\cos(\alpha_n x)}{\sqrt{k^2-\alpha_n^2}}+\sum_{n=n_1+1}^{\infty}\frac{\sin(\alpha_n x)}{\sqrt{\alpha_n^2-k^2}} +\sum_{n=1}^{n_2}\frac{\cos(\alpha_{-n}x)}{\sqrt{k^2-\alpha_{-n}^2}}+\sum_{n=n_2+1}^{\infty}\frac{\sin(\alpha_{-n}x)}{\sqrt{\alpha_{-n}^2-k^2}}\right\}, \tag{12}$$

and

$$Y_0(kx)+S_0^Y J_0(kx)+2\sum_{\ell=1}^{\infty}S_{2\ell}^Y J_{2\ell}(kx)+2\sum_{\ell=0}^{\infty}S_{2\ell+1}^J J_{2\ell+1}(kx)=\frac{2}{d}\left\{\frac{\sin(\alpha_0 x)}{\chi_0}+\sum_{n=1}^{n_1}\frac{\sin(\alpha_n x)}{\sqrt{k^2-\alpha_n^2}}-\sum_{n=n_1+1}^{\infty}\frac{\cos(\alpha_n x)}{\sqrt{\alpha_n^2-k^2}} +\sum_{n=1}^{n_2}\frac{\sin(\alpha_{-n}x)}{\sqrt{k^2-\alpha_{-n}^2}}-\sum_{n=n_2+1}^{\infty}\frac{\cos(\alpha_{-n}x)}{\sqrt{\alpha_{-n}^2-k^2}}\right\}. \tag{13}$$

By solving these equations for the lattice sums we obtain the formulas (A1), (A9), and (A10) for S_ℓ^J, the formula (A4) for S_0^Y, and the recurrence relations (A13) and (A14) for S_ℓ^Y. (See Appendix A.) Due to the length of these formulas we have presented them only in the Appendix A.

B. Lattice sum identities

An alternative method of evaluating lattice sums is provided by the method of lattice sum identities. These have previously been discussed only in the context of lattice sums for Laplace's equation [10], and for doubly-periodic systems with normally-incident radiation [11]. The extension reported here to the Helmholtz equation for an off-axis incidence requires a substantial generalization of the symmetry arguments used previously.

The definition of the lattice sums (7) may be generalized for an arbitrary origin. If we choose the reference point at $(d/2,0)$, the corresponding definition for the lattice sums is

$$s_\ell^+(\alpha_0,k,d)=\sum_{n=-\infty}^{\infty}H_\ell^{(1)}(k|nd-d/2|)e^{i\ell\varphi_n}e^{i\alpha_0 nd}, \tag{14}$$

where $\varphi_0=\pi$, while the lattice sums evaluated with respect to the point $(-d/2,0)$ are given by the formula:

$$s_\ell^-(\alpha_0,k,d)=\sum_{n=-\infty}^{\infty}H_\ell^{(1)}(k|nd+d/2|)e^{i\ell\varphi_n}e^{i\alpha_0 nd}, \tag{15}$$

where $\varphi_0=0$.

The two quantities, defined in (14) and (15), satisfy the relation:

$$s_\ell^+(\alpha_0,k,d)=e^{i\alpha_0 d}\,s_\ell^-(\alpha_0,k,d)\ , \tag{16}$$

which follows from their definition.

We express the lattice sums s_ℓ^+ and s_ℓ^- in terms of the lattice sums (7). This leads us to the lattice sum identities (C13) and (C15) for the lattice sums S_ℓ^J and S_ℓ^Y, respectively (see Appendix C). In what follows we will use (C13) and (C15) to evaluate the lattice sums.

In the case of normal incidence ($\alpha_0=0$), all the lattice sums of odd order vanish [7], and we obtain the lattice sum identities:

$$J_{2\ell-1}(kd/2)+S_0^J J_{2\ell-1}(kd/2) +\sum_{m=1}^{\infty}\left[J_{2\ell-1-2m}(kd/2)+J_{2\ell-1+2m}(kd/2)\right]S_{2m}^J=0, \tag{17}$$

$$Y_{2\ell-1}(kd/2) + S_0^Y J_{2\ell-1}(kd/2) + \sum_{m=1}^{\infty} [J_{2\ell-1-2m}(kd/2) + J_{2\ell-1+2m}(kd/2)]\, S_{2m}^Y = 0. \quad (18)$$

The first equation is identically satisfied by the expression [7]:

$$S_{2\ell}^J = -\delta_{\ell,0} + \frac{2}{kd} + \frac{4}{d}\sum_{n=1}^{n_1} \frac{\cos[2\ell \arcsin(nK/k)]}{\sqrt{k^2-(nK)^2}}, \quad (19)$$

where $2\pi n_1 < kd < 2\pi(n_1+1)$.

III. THE QUASIPERIODIC GREEN'S FUNCTION

A. Green's function in terms of lattice sums

The Green's function, given by (2) or (3), is quasiperiodic and satisfies the relation:

$$G(d/2, y; \alpha_0) = e^{i\alpha_0 d} G(-d/2, y; \alpha_0)\ , \ \forall y \in [0, \infty). \quad (20)$$

Within the domain defined by $-d/2 \leq x \leq d/2$ and $-d/2 \leq y \leq d/2$, we may apply Graf's addition theorem for the Hankel functions and expand (2) in terms of Bessel functions:

$$G(x,y;\alpha_0) = \frac{1}{4i}\left[H_0^{(1)}(kr) + \sum_{\ell=-\infty}^{\infty} S_\ell J_\ell(kr) e^{-i\ell\theta}\right] = \frac{1}{4i}\left[H_0^{(1)}(kr) + S_0 J_0(kr) + 2\sum_{\ell=1}^{\infty} S_\ell J_\ell(kr)\cos(\ell\theta)\right], \quad (21)$$

where r and θ are the polar coordinates in the xy plane. In this way, the Green's function for off-axis incidence is represented as a Neumann series with coefficients given by the lattice sums.

The sources of the Green's function (21) are located at $x = 0$ [represented by $H_0^{(1)}(kr)$] and $x = nd$, with $n = \pm1, \pm2, \ldots$ (represented by the series). Therefore, the radius of convergence of the series in (21) is $r = d$. These physical arguments are supported, mathematically, by the asymptotic estimates for the S_ℓ^Y with large ℓ, given by the nearest-neighbors approximation:

$$S_{2\ell}^Y \approx 2Y_{2\ell}(kd)\cos(\alpha_0 d)\,, \quad (22)$$

$$S_{2\ell-1}^Y \approx 2Y_{2\ell-1}(kd)\sin(\alpha_0 d)\,. \quad (23)$$

The lattice sums S_ℓ^J are bounded for all ℓ. Thus, the convergence radius of the series (21) follows from the convergence criteria for Neumann series [12].

Substituting (9) and (10) in (21), we obtain the real and imaginary parts of the Green's function:

$$\mathrm{Re}[G(x,y;\alpha_0)] = \frac{1}{4}\left\{Y_0(kr) + S_0^Y J_0(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}^Y J_{2\ell}(kr)\cos(2\ell\theta) + 2\sum_{\ell=1}^{\infty} S_{2\ell-1}^J J_{2\ell-1}(kr)\cos[(2\ell-1)\theta]\right\}, \quad (24)$$

$$\mathrm{Im}[G(x,y;\alpha_0)] = -\frac{1}{4}\left\{J_0(kr) + S_0^J J_0(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}^J J_{2\ell}(kr)\cos(2\ell\theta) - 2\sum_{\ell=1}^{\infty} S_{2\ell-1}^Y J_{2\ell-1}(kr)\cos[(2\ell-1)\theta]\right\}. \quad (25)$$

We mention that, in the case of normal incidence ($\alpha_0 = 0$), when all the lattice sums of odd order vanish, these equations become

$$\mathrm{Re}[G(x,y;0)] = \frac{1}{4}\left\{Y_0(kr) + S_0^Y J_0(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}^Y J_{2\ell}(kr)\cos(2\ell\theta)\right\}, \quad (26)$$

$$\mathrm{Im}[G(x,y;0)] = -\frac{1}{4}\left\{J_0(kr) + S_0^J J_0(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}^J J_{2\ell}(kr)\cos(2\ell\theta)\right\}. \quad (27)$$

By substituting (19) in (27), we obtain

$$\mathrm{Im}[G(x,y;0)] = -\frac{1}{2d}\sum_{n=-n_1}^{n_1} \frac{\cos(nKx)\cos(\chi_n y)}{\chi_n}. \quad (28)$$

Consequently, the imaginary part of the Green's function is bounded and the sources of the Green's function are represented by the real part only. At the same time, the imaginary part of the Green's function is related with propagating waves, while the real part is related with evanescent waves.

In particular, for incident radiation with the wavelength $\lambda > d$ ($kd < 2\pi$; i.e., $n_1 = 0$), from (28), we find that the imaginary part of the Green's function is independent of x:

$$\mathrm{Im}\,[G(x,y;0)] = -\frac{1}{2kd}\cos{(ky)}\,.$$

In the case of oblique incidence we obtain a decomposition of the Green's function, for propagating and evanescent waves, of the form

$$G(x,y;\alpha_0) = G_{\mathrm{PW}}(x,y;\alpha_0) + G_{\mathrm{EW}}(x,y;\alpha_0)\,, \qquad (29)$$

where

$$G_{\mathrm{PW}}(x,y;\alpha_0) = \frac{1}{2id}\sum_{n=-n_2}^{n_1} \frac{e^{i\alpha_n x}\cos{(\chi_n y)}}{\chi_n}\,, \qquad (30)$$

$$G_{\mathrm{EW}}(x,y;\alpha_0) = \frac{1}{4}\Bigg\{ Y_0(kr) + S_0^Y J_0(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}^Y J_{2\ell}(kr)\cos{(2\ell\theta)} + 2i\sum_{\ell=1}^{\infty} S_{2\ell-1}^Y J_{2\ell-1}(kr)\cos{[(2\ell-1)\theta]}\Bigg\}\,. \qquad (31)$$

In Figs. 1 and 2 we display graphs of the real and imaginary parts of the functions G, G_{PW}, and G_{EW}. It can be seen that for $\lambda < d$ (Fig. 1) the behavior of the Green's function is dominated by the propagating waves. The minimum exhibited by the function G_{EW} at $x = 0$ is generated by the term $Y_0(kr)$ in (31). As $|y|$ tends to zero, this minimum becomes a logarithmic singularity, describing the source at the origin.

In Fig. 2, $\lambda > d$ and the behavior of the Green's function is dominated by the evanescent waves. This creates a more pronounced minimum of Re$[G]$, at $x = 0$, for the same value of $|y|$ as in Fig. 1.

In both cases ($\lambda < d$ and $\lambda > d$), the asymmetries of the Green's function (in amplitude and phase), with respect to the reflection $x \to -x$, are due to the fact that G_{EW} is in phase or antiphase with G_{PW}. Therefore, the decomposition (29) of the Green's function is interesting for physical interpretations.

B. Symmetry properties of the Green's function

From the expression (2) we find that, in addition to (20), the Green's function satisfies the relation:

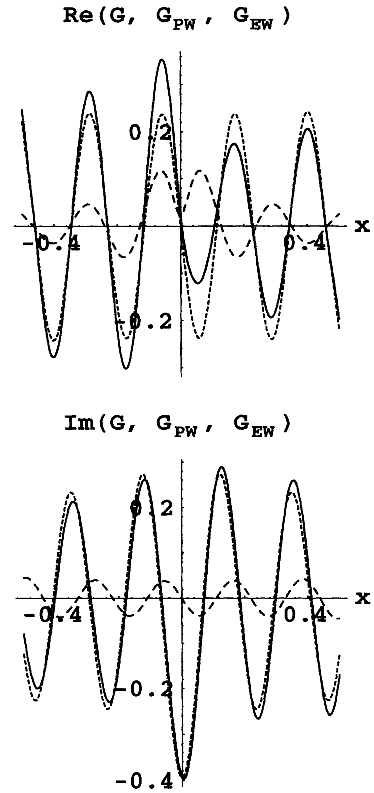

FIG. 1. The case of a radiation with $\lambda = 0.23$, incident at an angle $\theta_i = \pi/8$ on a grating with $d = 1$. The real and imaginary parts of the Green's function G (solid curves) and its components G_{PW} (thin dashed curves) and G_{EW} (thick dashed curves), for $|y| = 0.03$.

$$G(d/2,y;\alpha_0) = e^{i\alpha_0 d}\,G(d/2,y;-\alpha_0)\ ,\ \forall y \in [0,\infty). \quad (32)$$

We may split the Green's function into two parts; one of them symmetric with respect to the transform $\alpha_0 \to -\alpha_0$, and the other antisymmetric with respect to the same transform:

$$G(x,y;\alpha_0) = G_s(x,y;\alpha_0) + G_a(x,y;\alpha_0)\ .$$

The lattice sums satisfy the relations (C9) and (C10), so that, from (21), we deduce

$$G_s(x,y;\alpha_0) = \frac{1}{4i}\left[H_0^{(1)}(kr) + S_0 J_0(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}J_{2\ell}(kr)\cos{(2\ell\theta)}\right], \qquad (33)$$

$$G_a(x,y;\alpha_0) = \frac{1}{2i}\sum_{\ell=1}^{\infty} S_{2\ell-1}J_{2\ell-1}(kr)\cos{[(2\ell-1)\theta]}. \qquad (34)$$

As well, these two functions are symmetric and antisymmetric, respectively, under the reflection $x \to -x$:

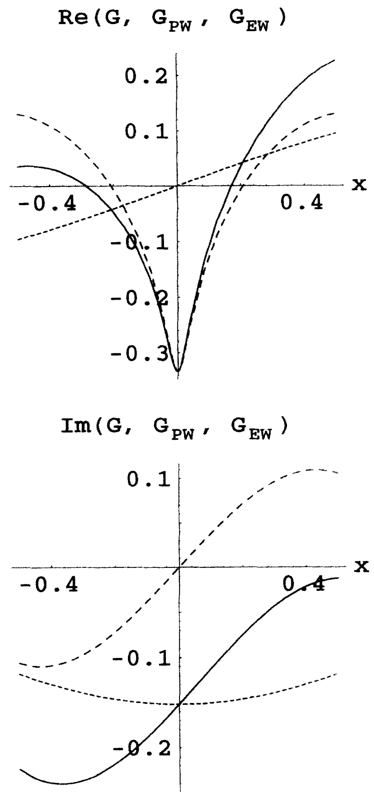

FIG. 2. The case of a radiation with $\lambda = 1.77$, incident at an angle $\theta_i = \pi/8$ on a grating with $d = 1$. The real and imaginary parts of the Green's function G (solid curves) and its components $G_{\rm PW}$ (thin dashed curves) and $G_{\rm EW}$ (thick dashed curves), for $|y| = 0.03$.

$$G_s(x,y;\alpha_0) = G_s(x,y;-\alpha_0) = G_s(-x,y;\alpha_0) = G_s(-x,y;-\alpha_0)\,,$$

$$G_a(x,y;\alpha_0) = -G_a(x,y;-\alpha_0) = -G_a(-x,y;\alpha_0) = G_a(-x,y;-\alpha_0)\,,$$

so that, the Green's function is invariant with respect to the combined transform ($x \to -x$, $\alpha_0 \to -\alpha_0$).

We choose a point $\mathbf{r} = (d/2)\hat{\mathbf{x}} + y\hat{\mathbf{y}}$, located on the symmetry line $x = d/2$ ($\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ represent the unit vectors along the x and y axis, respectively). For $y \in [-d/2, d/2]$, by substituting in (33) and (34) the series expansions:

$$H_0^{(1)}[k|(d/2)\hat{\mathbf{x}} + y\hat{\mathbf{y}}|] = \sum_{m=-\infty}^{\infty} H_{2m}^{(1)}(kd/2) J_{2m}(ky)(-1)^m,$$

$$J_0[k|(d/2)\hat{\mathbf{x}} + y\hat{\mathbf{y}}|] = \sum_{m=-\infty}^{\infty} J_{2m}(kd/2) J_{2m}(ky)(-1)^m,$$

$$J_\ell[k|(d/2)\hat{\mathbf{x}} + y\hat{\mathbf{y}}|]\cos(\ell\theta) = \sum_{m=-\infty}^{\infty} J_{\ell-2m}(kd/2) J_{2m}(ky)(-1)^m,$$

and by using the lattice sum identity (C11), we obtain

$$G_a(d/2,y;\alpha_0) = i\,\tan\left(\frac{\alpha_0 d}{2}\right) G_s(d/2,y;\alpha_0)\,, \quad \forall y \in [-d/2, d/2]\,. \tag{35}$$

Consequently, along the symmetry line $x = d/2$, the Green's function may be written in the form

$$G(d/2,y;\alpha_0) = \left[1 + i\,\tan\left(\frac{\alpha_0 d}{2}\right)\right] G_s(d/2,y;\alpha_0)\,. \tag{36}$$

The lattice sum identities (C8) and the symmetry relation (35) are equivalent. The quasiperiodicity relation (20) follows from anyone of them.

We mention that, for $x = 0$, the antisymmetric part of the Green's function vanishes, and the Green's function exhibits a logarithmic singularity at the origin.

As the decomposition of the Green's function into the symmetric and antisymmetric parts is very suitable for numerical calculations (discussed below), we mention the relation between these components of the Green's function and the decomposition (29):

$$G_{\rm PW}(x,y;\alpha_0) = {\rm Re}[G_a(x,y;\alpha_0)] + i\,{\rm Im}[G_s(x,y;\alpha_0)],$$
$$G_{\rm EW}(x,y;\alpha_0) = {\rm Re}[G_s(x,y;\alpha_0)] + i\,{\rm Im}[G_a(x,y;\alpha_0)].$$

IV. NUMERICAL RESULTS

A. Evaluation of the lattice sums

The recurrence relations (A13) and (A14) become unstable, numerically, for lattice sums of order $\ell > kd$. One reason for this may be seen in the first two terms in square brackets on the right hand side, where we evaluate an inverse square root, and then subtract an increasing number of terms in its expansion.

Instead, we may use the linear system provided by the lattice sum identities (C15). In order to truncate this sytem, we make use of the fact that, for large orders, the lattice sums are well approximated by the nearest-neighbors estimates (22) and (23). By adding and subtracting the asymptotic series for S_ℓ^Y, in (C15), we obtain

$$\left[\cos(\alpha_0 d) - (-1)^{\ell}\right] \left\{ Y_\ell(kd/2) + \left[S_0^Y - 2Y_0(kd)\cos(\alpha_0 d)\right] J_\ell(kd/2) \right.$$

$$\left. + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] \left[S_{2m}^Y - 2Y_{2m}(kd)\cos(\alpha_0 d)\right] \right\}$$

$$- \sin(\alpha_0 d) \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] \left[S_{2m-1}^Y - 2Y_{2m-1}(kd)\sin(\alpha_0 d)\right] \right\}$$

$$+ \left[\cos(\alpha_0 d) - (-1)^{\ell}\right] \left\{ 2Y_0(kd)\cos(\alpha_0 d) J_\ell(kd/2) \right.$$

$$\left. + 2\sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] Y_{2m}(kd)\cos(\alpha_0 d) \right\}$$

$$- \sin(\alpha_0 d) \left\{ 2\sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] Y_{2m-1}(kd)\sin(\alpha_0 d) \right\} = 0 . \tag{37}$$

For the last two series, we get a closed form sum by means of Neumann's addition theorem [13]:

$$Y_\ell(k|d - d/2|) = \sum_{m=-\infty}^{\infty} Y_{\ell+m}(kd) J_m(kd/2) = \sum_{n=-\infty}^{\infty} Y_n(kd)(-1)^{\ell+n} J_{\ell-n}(kd/2) ,$$

$$Y_\ell(k|d + d/2|) = \sum_{m=-\infty}^{\infty} Y_{\ell-m}(kd) J_m(kd/2) = \sum_{n=-\infty}^{\infty} Y_n(kd) J_{\ell-n}(kd/2) .$$

Consequently, we have

$$Y_\ell(3kd/2) + (-1)^{\ell} Y_\ell(kd/2) = 2\sum_{m=-\infty}^{\infty} Y_{2m}(kd) J_{\ell-2m}(kd/2) ,$$

$$Y_\ell(3kd/2) - (-1)^{\ell} Y_\ell(kd/2) = 2\sum_{m=-\infty}^{\infty} Y_{2m-1}(kd) J_{\ell-2m+1}(kd/2) ,$$

and (37) takes the form

$$[\cos(\alpha_0 d) - (-1)^{\ell}] \left\{ Y_\ell(3kd/2)\cos(\alpha_0 d) + [S_0^Y - 2Y_0(kd)\cos(\alpha_0 d)] J_\ell(kd/2) \right.$$

$$\left. + \sum_{m=1}^{\infty} [J_{\ell-2m1}(kd/2) + J_{\ell+2m1}(kd/2)][S_{2m1}^Y - 2Y_{2m1}(kd)\cos(\alpha_0 d)] \right\} - \sin(\alpha_0 d) \left\{ Y_l(3kd/2)\sin(\alpha_0 d) \right.$$

$$\left. + \sum_{m=1}^{\infty} [J_{l-2m+1}(kd/2) - J_{l+2m-1}(kd/2)][S_{2m-1}^Y - 2Y_{2m-1}(kd)\sin(\alpha_0 d)] \right\} = 0. \tag{38}$$

We introduce the new unknowns:

$$x_\ell = \frac{1}{2} \left\{ \frac{S_\ell^Y}{Y_\ell(kd)} - \left[1 + (-1)^{\ell}\right]\cos(\alpha_0 d) - \left[1 - (-1)^{\ell}\right]\sin(\alpha_0 d) \right\} ,$$

and truncate (38) to the order N:

$$2[\cos(\alpha_0 d) - (-1)^{\ell}] \left\{ Y_0(kd) J_\ell(kd/2) x_0 + \sum_{m=1}^{N} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] Y_{2m}(kd) x_{2m} \right\}$$

$$-2\sin(\alpha_0 d) \left\{ \sum_{m=1}^{N} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] Y_{2m-1}(kd) x_{2m-1} \right\}$$

$$= \left\{ - \left[\cos(\alpha_0 d) - (-1)^{\ell}\right] \cos(\alpha_0 d) + \sin^2(\alpha_0 d) \right\} Y_\ell(3kd/2) . \tag{39}$$

This method of truncation assumes that for $\ell \geq N+1$ the equations (22) and (23) are exact; i.e., $x_\ell = 0$, for $\ell \geq N+1$. Consequently, the accuracy of the values of the lattice sums, obtained by this method, depends on how close the lattice sums of order larger than N are to their nearest-neighbors estimate. But, at the same time, too large a system of the form (39) is ill conditioned. This is due to the fact that the lattice sums S_ℓ^Y, of high order ℓ, become large (see Tables I and II).

In order to avoid these difficulties we choose a hybrid technique: first we evaluate M lattice sums using the recurrence relations (A13) and (A14), then, we solve the system (39) for the unknowns $\{x_M, \ldots, x_N\}$. The lattice sums of order larger N are given by (22) and (23).

In the Tables I and II we display the results from the hybrid method in different cases. These numerical results were obtained with a MATHEMATICA program run on a SPARC-10 computer workstation. The precision was of 32 digits for the recurrence relation and 16 digits for the lattice sums identities.

In Table I, for a short wavelength ($\lambda = 0.23$), we evaluated the first 12 lattice sums S_ℓ^Y by means of the recurrence relations (A13)–(A14). From the first column it can be seen that the number of significant digits decreases rapidly for $\ell > 14$ and the algorithm fails completely for $\ell > 21$. With the first 12 lattice sums ($M = 11$) we solved the system (39) for the lattice sums $\{S_{12}^Y, \ldots, S_{49}^Y\}$. The numerical results show a good agreement between the lattice sums given by (A13) and (A14) and the lattice sums from (39) for $\ell = 12, \ldots, 17$, the relative error being less than 10^{-5}. Actually, a direct comparison with numerically-evaluated partial sums of high orders in (9) and (10) shows the validity of the results from (39). For $\ell > 43$ we have a relative error less than 10^{-5} between the results from (39) and the nearest-neighbors estimate (22) and (23). We may say that the lattice sum identities are filling the gap between the highest-order lattice sums, which can be obtained (with high accuracy) from the recurrence relation, and the lattice sums of order $\ell > kd$, for which we may use the nearest-neighbors estimate.

Trying to solve the lattice sum identities directly for all the lattice sums $\{S_0^Y, \ldots, S_{49}^Y\}$, we obtained a strongly ill-conditioned matrix of the linear system (39), which gave inaccurate numerical results. In this particular case, the values of the lattice sums for $\ell < kd$ are less than 1, while starting with $\ell \sim kd$, the corresponding values increase rapidly. The rapidly increasing dynamic range of the elements of the matrix then renders a numerical solution difficult.

The gap between the highest order of the lattice sums, for which the recurrence relation may be used, and the order, from which we may use the nearest-neighbors estimate, becomes smaller as λ increases and almost vanishes for $\lambda > d$ (see Table II). At the same time, we may ob-

TABLE I. Off-axis incidence at $\theta_i = \pi/8$ for $\lambda = 0.23$ and $d = 1$. The first 50 values of $S_\ell^Y(\alpha_0, k, d)$ obtained by the hybrid technique. The columns labeled by RR, LSI, and NNE represent the results from the recurrence relation, lattice sum identities, and nearest-neighbors estimate, respectively.

ℓ	RR	LSI	NNE	ℓ	LSI	NNE
0	0.16104658		−0.15490169	25	−0.73723782	0.08729420
1	−0.15571020		0.04092682	26	−0.84071354	0.15349761
2	−0.17175436		0.15670328	27	1.25296581	0.39864653
3	0.21469466		−0.00276611	28	1.25235165	0.32030707
4	0.20898202		−0.15706857	29	−0.27214775	0.69337924
5	−0.33567720		−0.07373322	30	−0.21206723	0.56484202
6	−0.28765032		0.14083998	31	2.32434610	1.36989324
7	0.51161439		0.17662615	32	1.90261541	1.30453117
8	0.42758564		−0.08641471	33	3.04452690	3.71302066
9	−0.70236456		−0.26080170	34	3.54658672	4.08919537
10	−0.63440080		−0.01690913	35	1.35236736×10^1	1.32157376×10^1
11	0.82304881		0.24021297	36	1.68887646×10^1	1.62721770×10^1
12	0.86221953	0.86221953	0.13322440	37	5.78366481×10^1	5.81116788×10^1
13	−0.79590391	−0.79590391	−0.04555448	38	7.78280644×10^1	7.83761061×10^1
14	−0.99299669	−0.99299669	−0.15929326	39	3.05006107×10^2	3.04528242×10^2
15	0.6940737	0.69407376	−0.22598549	40	4.44594709×10^2	4.44428948×10^2
16	0.925426	0.92542628	0.01007588	41	1.85977359×10^3	1.86003691×10^3
17	−0.80574	−0.80574556	0.24561508	42	2.91269330×10^3	2.91258398×10^3
18	−0.7898	−0.78977182	0.17372668	43	1.30344632×10^4	1.30348112×10^4
19	1.234	1.23405074	0.13514144	44	2.17605509×10^4	2.17603499×10^4
20	0.92	0.92086218	−0.06069772	45	1.03546461×10^5	1.03545949×10^5
21	−1.3	−1.32456842	−0.28295378	46	1.83351911×10^5	1.83352667×10^5
22		−1.18802661	−0.20086894	47	9.23413193×10^5	9.23413734×10^5
23		0.66196236	−0.25512245	48	1.72712539×10^6	1.72712420×10^6
24		0.93854254	−0.05743088	49	9.17081576×10^6	9.17081491×10^6

TABLE II. Off-axis incidence at $\theta_i = \pi/8$. The first 30 values of $S_\ell^Y(\alpha_0, k, d)$ obtained by the hybrid technique for $\lambda < d$ and $\lambda > d$ $(d = 1)$. The columns labeled by RR, LSI, and NNE represent the results from the recurrence relation, lattice sum identities, and nearest-neighbors estimate, respectively.

	$\lambda = 0.46$			$\lambda = 1.77$		
ℓ	RR	LSI	NNE	RR	LSI	NNE
0	0.360931		0.062430	0.163655		0.071023
1	−0.089475		0.355328	0.437841		0.807986
2	−0.418275		−0.091856	0.028366		0.027118
3	0.218864		−0.307767	−0.354132		−0.666248
4	0.586162		0.168317	−0.517756		−0.269894
5	−0.560586		0.133463	−2.080086		−2.155066
6	−0.817395	−0.817395	−0.223579	−1.014262	−1.014262	−1.038923
7	1.154748	1.154748	0.213834	-1.461940×10^1	-1.461940×10^1	-1.413538×10^1
8	0.978117	0.978117	0.099622	-1.009441×10^1	-1.009441×10^1	-1.097967×10^1
9	−1.647013	−1.647013	−0.420164	-2.163098×10^2	-2.163098×10^2	-2.154150×10^2
10	−1.056687	−1.056687	0.213533	-2.208925×10^2	-2.208925×10^2	-2.245072×10^2
11	1.330980	1.330980	−0.132655	-5.654732×10^3	-5.654733×10^3	-5.651758×10^3
12	1.599493	1.599493	−0.092692	-7.306239×10^3	-7.306236×10^3	-7.326839×10^3
13	−1.144024	−1.144024	0.420621	-2.241451×10^5	-2.241451×10^5	-2.241200×10^5
14	−2.327877	−2.327877	−0.360135	-3.463669×10^5	-3.463672×10^5	-3.465662×10^5
15	2.471472	2.471472	0.884683	-1.245601×10^7	-1.245602×10^7	-1.245569×10^7
16	1.19337	1.193368	−0.738811	-2.2344×10^7	-2.234435×10^7	-2.234724×10^7
17	0.3802	0.380201	2.175673	-9.22×10^8	-9.219702×10^8	-9.219651×10^8
18	−4.03	−4.032610	−2.324140	-1.881×10^9	-1.881359×10^9	-1.881410×10^9
19	11.	10.925802	8.654941	-8.758×10^{10}	-8.758049×10^{10}	-8.758034×10^{10}
20		−9.552479	-1.129392×10^1	-2.002×10^{11}	-2.002362×10^{11}	-2.002381×10^{11}
21		4.747525×10^1	4.982314×10^1	-1.0378×10^{13}	-1.037829×10^{13}	-1.037829×10^{13}
22		-7.743048×10^1	-7.535197×10^1		-2.627217×10^{13}	-2.627216×10^{13}
23		3.809760×10^2	3.793531×10^1		-1.500109×10^{15}	-1.500109×10^{15}
24		-6.451198×10^2	-6.471999×10^2		-4.164540×10^{15}	-4.164547×10^{15}
25		3.640365×10^3	3.641961×10^3		-2.597026×10^{17}	-2.597026×10^{17}
26		-6.894904×10^3	-6.892827×10^3		-7.844496×10^{17}	-7.844493×10^{17}
27		4.275678×10^4	4.275495×10^4		-5.304149×10^{19}	-5.304148×10^{19}
28		-8.870288×10^4	-8.870494×10^4		-1.731668×10^{20}	-1.731668×10^{20}
29		6.002649×10^5	6.002646×10^5		-1.261826×10^{22}	-1.261826×10^{22}

tain a high accuracy by using the recurrence relation only to evaluate the first six lattice sums, and the lattice sum identities for the remaining 23. This gives a matrix of reduced size in the linear system (39), and avoids inversion of ill-conditioned matrices.

B. The Green's function

The main advantage of using the lattice sums method is that, for a given problem of electromagnetic scattering by a grating, defined by (k, d, α_0), the coefficients of the series (21) have to be evaluated once only. This increases appreciably the speed of numerical evaluation of the Green's function at any point in the xy plane.

After substituting (9) and (10) in (33) and (34), we use the fact that the series involving the S_ℓ^J have the closed-form sums:

$$2\sum_{\ell=1}^{\infty} S_{2\ell-1}^J J_{2\ell-1}(kr)\cos\left[(2\ell-1)\theta\right] = \frac{2}{d}\sum_{n=-n_2}^{n_1} \frac{\cos(\chi_n y)\sin(\alpha_n x)}{\chi_n},$$

$$J_0(kr) + S_0^J J_0(kr) + 2\sum_{\ell=1}^{\infty} S_{2\ell}^J J_{2\ell}(kr)\cos(2\ell\theta) = \frac{2}{d}\sum_{n=-n_2}^{n_1} \frac{\cos(\chi_n y)\cos(\alpha_n x)}{\chi_n}.$$

These formulas are obtained by direct substitution of (A9) and (A10) in the corresponding series.

For numerical calculations, we may accelerate the series containing the S_ℓ^Y by means of Kummer's method. Therefore, we add and subtract the asymptotic series given by (22) and (23). Then, we use the relations:

$$Y_0(k|\mathbf{r} - d\hat{\mathbf{x}}|) + Y_0(k|\mathbf{r} + d\hat{\mathbf{x}}|) = 2\sum_{\ell=-\infty}^{\infty} Y_{2\ell}(kd) J_{2\ell}(kr)\cos(2\ell\theta),$$

$$Y_0(k|\mathbf{r}-d\hat{\mathbf{x}}|)-Y_0(k|\mathbf{r}+d\hat{\mathbf{x}}|) = 2\sum_{\ell=-\infty}^{\infty} Y_{2\ell-1}(kd)J_{2\ell-1}(kr)\cos[(2\ell-1)\theta],$$

which are valid for $|\mathbf{r}| < d$.

Finally, we truncate the remaining series to order N, so that the symmetric and antisymmetric parts of the Green's function take the form

$$4G_s(x,y;\alpha_0) = Y_0(kr) + \left[S_0^Y - 2Y_0(kd)\cos(\alpha_0 d)\right]J_0(kr) + 2\sum_{\ell=1}^{N}\left[S_{2\ell}^Y - 2Y_{2\ell}(kd)\cos(\alpha_0 d)\right]J_{2\ell}(kr)\cos(2\ell\theta) + [Y_0(k|\mathbf{r}-d\hat{\mathbf{x}}|)+Y_0(k|\mathbf{r}+d\hat{\mathbf{x}}|)]\cos(\alpha_0 d) - i\frac{2}{d}\sum_{n=-n_2}^{n_1}\frac{\cos(\alpha_n x)\cos(\chi_n y)}{\chi_n}, \quad (40)$$

$$4G_a(x,y;\alpha_0) = \frac{2}{d}\sum_{n=-n_2}^{n_1}\frac{\sin(\alpha_n x)\cos(\chi_n y)}{\chi_n} + 2i\sum_{\ell=1}^{N}\left[S_{2\ell-1}^Y - 2Y_{2\ell-1}(kd)\sin(\alpha_0 d)\right] \times J_{2\ell-1}(kr)\cos[(2\ell-1)\theta] + i[Y_0(k|\mathbf{r}+d\hat{\mathbf{x}}|)+Y_0(k|\mathbf{r}+d\hat{\mathbf{x}}|)]\sin(\alpha_0 d). \quad (41)$$

and the Green's function may be evaluated from

$$G(x,y;\alpha_0) = G_s(x,y;\alpha_0) + G_a(x,y;\alpha_0). \quad (42)$$

The symmetry properties of the Green's function imply that

$$G(-x,y;\alpha_0) = G_s(x,y;\alpha_0) - G_a(x,y;\alpha_0).$$

Therefore, the Green's function in the range $x \in [-d/2, 0)$ is completely determined by the knowledge of the Green's function in the range $x \in (0, d/2]$.

In Table III, the timing (T_1) for Eq. (42) represents the time to evaluate the Green's function for the first point (x,y). To do this, a set of lattice sums S_ℓ^Y up to the order $n = N-1$ has to be evaluated. (For the case of Table III, the CPU time required to evaluate 12 lattice sums from the recurrence relation was 878 s, while the corresponding time for the next 38 sums from the lattice sum identities was 353 s, giving a total of 1231 s.) All other subsequent evaluations of the Green's function, at any other point (x,y), in the table, use this set, and so require far less computation time.

The use of Eq. (3) for $|y| \geq 0.03$ is computationally advantageous, whereas for $|y| \leq 0.003$, Eq. (42) is superior if more than 30 Green's function evaluations are required. The lines labeled $O(1/n^3)$ represent the cubically-convergent series of the spectral domain form for the Green's function [7]. We stopped this series and the series in (3) when the relative difference of two successive partial sums was less than 10^{-15}. From (42) we obtain a very good approximation of these results summing only a reduced number of terms.

TABLE III. Off-axis incidence at $\theta_i = \pi/8$. Comparison between different numerical methods to evaluate the Green's function ($d = 1$). In the first column $O(1/n^3)$ represents the cubically-convergent form of (3). 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 computer CPU time, in seconds, required for n independent evaluations.

Eq.	λ	x	y	Re[$G(x,y)$]	Im[$G(x,y)$]	N	T_1	T_{50}	T_{100}
(3)	0.23	0.2	0.03	0.117120006144932	-0.108131857633201	154	4	225	407
$O(1/n^3)$				0.117120006144931	-0.108131857633201	121	8	372	725
(42)				0.117120006141860	-0.108131857633197	25	1232	1288	1347
(3)	0.23	0.2	0.003	0.115891895634567	-0.103497063599642	1386	36	1818	3855
$O(1/n^3)$				0.115891895634567	-0.103497063599643	836	48	2433	4649
(42)				0.115891895630095	-0.103497063599643	25	1232	1288	1345
(3)	0.23	0.2	0.0003	0.115881138140449	-0.103450147416784	12681	366	16904	33577
$O(1/n^3)$				0.115881138140448	-0.103450147416785	5416	301	15353	31959
(42)				0.115881138135960	-0.103450147416785	25	1232	1292	1349

V. CONCLUSIONS

We have presented methods for evaluating to high accuracy lattice sums for the Helmholtz equation in the case of diffraction gratings. We have shown how these lattice sums provide a computationally efficient way of evaluating the corresponding free-space Green's function $G(x, y; \alpha_0)$, when results of high accuracy are required for small values of $|y|$. The generalization of our methods to the calculation of Green's function in dielectric and lossy materials will be the object of future work.

The methods we have described involve complicated intermediate formulas, but their results are not difficult to implement numerically. We will be happy to provide on request copies of the MATHEMATICA implementation of our method. Its implementation in languages such as FORTRAN should provide no great problems.

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APPENDIX A: RECURRENCE RELATIONS FOR THE LATTICE SUMS

We obtain the same pair of equations, as (12) and (13), but for $-x$, if we consider $-d < x < 0$ in (6), with $\theta_x = \pi$. Therefore, (12) and (13) are valid for $x \in [-d, d] \setminus \{0\}$, i.e., x in the range $[-d, d]$ excluding the origin.

In the limit $x \to 0$, (12) leads us to the formula [8]

$$S_0^J = -1 + \frac{2}{d}\left[\frac{1}{\chi_0} + \sum_{n=1}^{n_1} \frac{1}{\sqrt{k^2 - \alpha_n^2}} + \sum_{n=1}^{n_2} \frac{1}{\sqrt{k^2 - \alpha_{-n}^2}}\right]. \qquad \text{(A1)}$$

To evaluate the same limit for (13), we replace Y_0 by the Neumann series [13]:

$$Y_0(kx) = \frac{2}{\pi}\left[\ln\left(\frac{kx}{2}\right) + \gamma\right] J_0(kx) - \frac{4}{\pi}\sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{\ell} J_{2\ell}(kx), \qquad \text{(A2)}$$

where γ is the Euler-Mascheroni constant, so that (13) becomes

$$\left\{S_0^Y + \frac{2}{\pi}\left[\ln\left(\frac{k|x|}{2}\right) + \gamma\right]\right\} J_0(kx) + 2\sum_{\ell=1}^{\infty}\left[S_{2\ell}^Y - \frac{2}{\pi}\frac{(-1)^\ell}{\ell}\right] J_{2\ell}(kx) + 2\sum_{\ell=0}^{\infty} S_{2\ell+1}^J J_{2\ell+1}(kx)$$

$$= \frac{2}{d}\left\{\frac{\sin(\alpha_0 x)}{\chi_0} + \sum_{n=1}^{n_1} \frac{\sin(\alpha_n x)}{\sqrt{k^2 - \alpha_n^2}} - \sum_{n=n_1+1}^{\infty} \frac{\cos(\alpha_n x)}{\sqrt{\alpha_n^2 - k^2}} + \sum_{n=1}^{n_2} \frac{\sin(\alpha_{-n} x)}{\sqrt{k^2 - \alpha_{-n}^2}} - \sum_{n=n_2+1}^{\infty} \frac{\cos(\alpha_{-n} x)}{\sqrt{\alpha_{-n}^2 - k^2}}\right\}. \qquad \text{(A3)}$$

In the right hand side, the sine functions tend to zero and for the remaining terms we apply the Kummer transform for series acceleration [13]. In the first series, we use the asymptotic form

$$\frac{1}{|\chi_n|} = \frac{1}{\sqrt{\alpha_n^2 - k^2}} \sim \frac{1}{nK} \text{ as } n \to \infty.$$

Then, we add and subtract the corresponding asymptotic series so that the series becomes

$$\sum_{n=n_1+1}^{\infty} \frac{\cos(\alpha_n x)}{\sqrt{\alpha_n^2 - k^2}} = \sum_{n=n_1+1}^{\infty}\left[\frac{\cos(\alpha_n x)}{\sqrt{\alpha_n^2 - k^2}} - \frac{1}{nK}\right] - \sum_{n=1}^{n_1} \frac{1}{nK} + \sum_{n=1}^{\infty} \frac{\cos(\alpha_n x)}{nK}.$$

We transform in the same way the second series in (A3). Finally, the zeroth-order approximation in x, and the substitutions $\alpha_n = \alpha_0 \pm nK$ and $K = 2\pi/d$, give us

$$-2\left\{\sum_{n=n_1+1}^{\infty}\left[\frac{1}{\sqrt{(2\pi n + \alpha_0 d)^2 - k^2 d^2}} - \frac{1}{2\pi n}\right] + \sum_{n=n_2+1}^{\infty}\left[\frac{1}{\sqrt{(2\pi n - \alpha_0 d)^2 - k^2 d^2}} - \frac{1}{2\pi n}\right] - \frac{1}{2\pi}\sum_{n=1}^{n_1}\frac{1}{n} - \frac{1}{2\pi}\sum_{n=1}^{n_2}\frac{1}{n}\right\}$$
$$- \frac{1}{\pi}\left\{\sum_{n=1}^{\infty} \frac{\cos[(nK + \alpha_0)x] + \cos[(nK - \alpha_0)x]}{n}\right\}_{(x\sim 0)}.$$

The last series may be expressed in terms of Clausen's function (see Appendix B) and, for small x, we obtain

$$-\frac{2}{\pi}\cos(\alpha_0 x)\sum_{n=1}^{\infty}\frac{\cos(nKx)}{n} = -\frac{2}{\pi}\cos(\alpha_0 x)\mathrm{Cl}_1(Kx) \approx \frac{2}{\pi}\ln\left(2\left|\sin\frac{Kx}{2}\right|\right) \approx \frac{2}{\pi}\ln(K|x|)$$

Finally, substituting in (A3) and with $J_\ell(0) = \delta_{\ell,0}$, we obtain the formula [8]

$$S_0^Y = -\frac{2}{\pi}\left[\ln\left(\frac{k}{2K}\right)+\gamma\right]+\frac{1}{\pi}\left[\sum_{n=1}^{n_1}\frac{1}{n}+\sum_{n=1}^{n_2}\frac{1}{n}\right]-2\left\{\sum_{n=n_1+1}^{\infty}\left[\frac{1}{\sqrt{(2\pi n+\alpha_0 d)^2-k^2d^2}}-\frac{1}{2\pi n}\right]\right.$$
$$\left.-\sum_{n=n_2+1}^{\infty}\left[\frac{1}{\sqrt{(2\pi n-\alpha_0 d)^2-k^2d^2}}-\frac{1}{2\pi n}\right]\right\}. \qquad \text{(A4)}$$

The two limits, (A1) and (A4), are the same for $x \to 0^+$ and $x \to 0^-$, which proves the continuity of the equations (12) and (A3) at $x = 0$. Consequently, these equations are defined over the whole interval $[-d, d]$. The symmetry properties of (12) and (A3), with respect to the reflection $x \to -x$, allow us to split them into four equations:

$$\left(S_0^J+1\right)J_0(kx)+2\sum_{\ell=1}^{\infty}S_{2\ell}^J J_{2\ell}(kx)=\frac{2}{d}\left\{\frac{\cos(\alpha_0 x)}{\chi_0}+\sum_{n=1}^{n_1}\frac{\cos(\alpha_n x)}{\sqrt{k^2-\alpha_n^2}}+\sum_{n=1}^{n_2}\frac{\cos(\alpha_{-n}x)}{\sqrt{k^2-\alpha_{-n}^2}}\right\}, \qquad \text{(A5)}$$

$$\sum_{\ell=0}^{\infty}S_{2\ell+1}^J J_{2\ell+1}(kx)=\frac{1}{d}\left\{\frac{\sin(\alpha_0 x)}{\chi_0}+\sum_{n=1}^{n_1}\frac{\sin(\alpha_n x)}{\sqrt{k^2-\alpha_n^2}}+\sum_{n=1}^{n_2}\frac{\sin(\alpha_{-n}x)}{\sqrt{k^2-\alpha_{-n}^2}}\right\}, \qquad \text{(A6)}$$

$$\left\{S_0^Y+\frac{2}{\pi}\left[\ln\left(\frac{k|x|}{2}\right)+\gamma\right]\right\}J_0(kx)+2\sum_{\ell=1}^{\infty}\left[S_{2\ell}^Y-\frac{2}{\pi}\frac{(-1)^\ell}{\ell}\right]J_{2\ell}(kx)$$
$$=-\frac{2}{d}\left\{\sum_{n=n_1+1}^{\infty}\frac{\cos(\alpha_n x)}{\sqrt{\alpha_n^2-k^2}}+\sum_{n=n_2+1}^{\infty}\frac{\cos(\alpha_{-n}x)}{\sqrt{\alpha_{-n}^2-k^2}}\right\}, \qquad \text{(A7)}$$

$$\sum_{\ell=0}^{\infty}S_{2\ell+1}^Y J_{2\ell+1}(kx)=-\frac{1}{d}\left\{\sum_{n=n_1+1}^{\infty}\frac{\sin(\alpha_n x)}{\sqrt{\alpha_n^2-k^2}}+\sum_{n=n_2+1}^{\infty}\frac{\sin(\alpha_{-n}x)}{\sqrt{\alpha_{-n}^2-k^2}}\right\}. \qquad \text{(A8)}$$

In the first two equations, $|\alpha_0|$ and $|\alpha_0 \pm nK|$ are less than k. Consequently, the general solutions are obtained by substituting in the right hand sides the Jacobi expansions [13]:

$$\cos(zx)=\cos\{kx\sin[\arcsin(z/k)]\}$$
$$=J_0(kx)+2\sum_{\ell=1}^{\infty}J_{2\ell}(kx)\cos[2\ell\arcsin(z/k)],$$

$$\sin(zx)=\sin\{kx\sin[\arcsin(z/k)]\}$$
$$=2\sum_{\ell=0}^{\infty}J_{2\ell+1}(kx)\sin[(2\ell+1)\arcsin(z/k)],$$

where z stands for α_0 and α_n, respectively. By equating the coefficients of the corresponding Bessel functions we obtain the general solutions of (A5) and (A6), in the form

$$S_{2\ell}^J=-\delta_{\ell,0}+\frac{2}{d}\left\{\frac{\cos[2\ell\arcsin(\alpha_0/k)]}{\sqrt{k^2-\alpha_0^2}}+\sum_{n=1}^{n_1}\frac{\cos[2\ell\arcsin(\alpha_n/k)]}{\sqrt{k^2-\alpha_n^2}}+\sum_{n=1}^{n_2}\frac{\cos[2\ell\arcsin(\alpha_{-n}/k)]}{\sqrt{k^2-\alpha_{-n}^2}}\right\}, \qquad \text{(A9)}$$

$$S_{2\ell+1}^J=\frac{2}{d}\left\{\frac{\sin[(2\ell+1)\arcsin(\alpha_0/k)]}{\sqrt{k^2-\alpha_0^2}}+\sum_{n=1}^{n_1}\frac{\sin[(2\ell+1)\arcsin(\alpha_n/k)]}{\sqrt{k^2-\alpha_n^2}}+\sum_{n=1}^{n_2}\frac{\sin[(2\ell+1)\arcsin(\alpha_{-n}/k)]}{\sqrt{k^2-\alpha_{-n}^2}}\right\}. \qquad \text{(A10)}$$

Now, let us consider first the right hand side of (A8). We expand

$$[(nK \pm \alpha_0)^2 - k^2]^{-1/2} = \frac{1}{nK}\sum_{s=0}^{\infty}\left(\pm i\frac{\chi_0}{nK}\right)^s P_s(\varphi) ,$$

where P_s are Legendre polynomials and $\varphi = i\alpha_0/\chi_0 = i\tan\theta_i$. By applying Kummer's method and expanding the sine functions we obtain the coefficient of x^{2N+1} in the form

$$-\frac{1}{d}\left\{\sum_{n=n_1+1}^{\infty}(-1)^N\frac{\alpha_n^{2N+1}}{(2N+1)!}\left[\frac{1}{\sqrt{\alpha_n^2-k^2}}-\frac{1}{nK}\sum_{s=0}^{2M+1}\left(i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right]\right.$$
$$\left.+\sum_{n=n_2+1}^{\infty}(-1)^N\frac{\alpha_{-n}^{2N+1}}{(2N+1)!}\left[\frac{1}{\sqrt{\alpha_{-n}^2-k^2}}-\frac{1}{nK}\sum_{s=0}^{2M+1}\left(-i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right]\right\}$$
$$+\frac{1}{2\pi}\left\{\sum_{n=1}^{n_1}(-1)^N\frac{\alpha_n^{2N+1}}{(2N+1)!n}\sum_{s=0}^{2M+1}\left(i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right.$$
$$\left.+\sum_{n=1}^{n_2}(-1)^N\frac{\alpha_{-n}^{2N+1}}{(2N+1)!n}\sum_{s=0}^{2M+1}\left(-i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right\}-\frac{c_{2N+1}}{\pi} .$$

Here, $M \geq N$ and c_{2N+1} is the coefficient of x^{2N+1} in the expression

$$\frac{1}{2}\left\{\sum_{n=1}^{\infty}\frac{\sin(\alpha_n x)}{n}\sum_{s=0}^{2M+1}\left(i\frac{\chi_0}{nK}\right)^s P_s(\varphi)+\sum_{n=1}^{\infty}\frac{\sin(\alpha_{-n}x)}{n}\sum_{s=0}^{2M+1}\left(-i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right\}$$
$$=\sum_{s=0}^{M}\left(i\frac{\chi_0}{K}\right)^{2s}P_{2s}(\varphi)\sin(\alpha_0 x)\,\mathrm{Cl}_{2s+1}(Kx)+\sum_{s=0}^{M}\left(i\frac{\chi_0}{K}\right)^{2s+1}P_{2s+1}(\varphi)\cos(\alpha_0 x)\,\mathrm{Cl}_{2s+2}(Kx) .$$

Substituting (B2) and (B3), and expanding the trigonometric functions we get

$$c_{2N+1}=(-1)^N\frac{\alpha_0^{2N+1}}{(2N+1)!}\sum_{n=0}^{N}\binom{2N+1}{2n}\left(\frac{K}{\alpha_0}\right)^{2n}\left\{-\sum_{s=0}^{n-1}\frac{B_{2n-2s}}{2n-2s}\left(i\frac{\chi_0}{K}\right)^{2s}P_{2s}(\varphi)\right.$$
$$\left.+[g(2n)-\ln(Kx)]\left(i\frac{\chi_0}{K}\right)^{2n}P_{2n}(\varphi)+\sum_{s=n+1}^{M}\left(i\frac{\chi_0}{K}\right)^{2s}P_{2s}(\varphi)\zeta(2s+1-2n)\right\}$$
$$+(-1)^N\frac{\alpha_0^{2N+1}}{(2N+1)!}\sum_{n=0}^{N}\binom{2N+1}{2n+1}\left(\frac{K}{\alpha_0}\right)^{2n+1}\left\{-\sum_{s=0}^{n-1}\frac{B_{2n-2s}}{2n-2s}\left(i\frac{\chi_0}{K}\right)^{2s+1}P_{2s+1}(\varphi)\right.$$
$$\left.+[g(2n+1)-\ln(Kx)]\left(i\frac{\chi_0}{K}\right)^{2n+1}P_{2n+1}(\varphi)+\sum_{s=n+1}^{M}\left(i\frac{\chi_0}{K}\right)^{2s+1}P_{2s+1}(\varphi)\zeta(2s+1-2n)\right\} . \tag{A11}$$

The Legendre polynomials satisfy the relation

$$\sum_{n=0}^{2N+1}\binom{2N+1}{n}\left(-\frac{1}{\varphi}\right)^n P_n(\varphi)=0 , \tag{A12}$$

so that the coefficient of the logarithm vanishes.

By equating the coefficients of x^{2N+1} in (A8) we obtain the recurrence relation

$$\left[\sum_{\ell=0}^{N}(-1)^{\ell}\binom{2N+1}{N-\ell}S_{2\ell+1}^{Y}\right]\left(\frac{k}{2}\right)^{2N+1}$$

$$=-\frac{1}{d}\left\{\sum_{n=n_1+1}^{\infty}\alpha_n^{2N+1}\left[\frac{1}{\sqrt{\alpha_n{}^2-k^2}}-\frac{1}{nK}\sum_{s=0}^{2M+1}\left(i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right]\right.$$
$$\left.+\sum_{n=n_2+1}^{\infty}\alpha_{-n}^{2N+1}\left[\frac{1}{\sqrt{\alpha_{-n}^2-k^2}}-\frac{1}{nK}\sum_{s=0}^{2M+1}\left(-i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right]\right\}$$

$$+\frac{1}{2\pi}\left\{\sum_{n=1}^{n_1}\frac{\alpha_n^{2N+1}}{n}\sum_{s=0}^{2M+1}\left(i\frac{\chi_0}{nK}\right)^s P_s(\varphi)+\sum_{n=1}^{n_2}\frac{\alpha_{-n}^{2N+1}}{n}\sum_{s=0}^{2M+1}\left(-i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right\}$$
$$-\frac{\alpha_0^{2N+1}}{\pi}\left\{\sum_{n=0}^{2N+1}\binom{2N+1}{n}\left(i\frac{\chi_0}{\alpha_0}\right)^n P_n(\varphi)\,g(n)-\sum_{n=0}^{N}\binom{2N+1}{2n}\left(\frac{K}{\alpha_0}\right)^{2n}F_n\right.$$
$$\left.-\sum_{n=0}^{N}\binom{2N+1}{2n+1}\left(\frac{K}{\alpha_0}\right)^{2n+1}G_n\right\}. \qquad \text{(A13)}$$

where

$$F_n=\sum_{s=0}^{n-1}\frac{B_{2n-2s}}{2n-2s}\left(i\frac{\chi_0}{K}\right)^{2s}P_{2s}(\varphi)-\sum_{s=n+1}^{M}\zeta(2s+1-2n)\left(i\frac{\chi_0}{K}\right)^{2s}P_{2s}(\varphi)\,,$$
$$G_n=\sum_{s=0}^{n-1}\frac{B_{2n-2s}}{2n-2s}\left(i\frac{\chi_0}{K}\right)^{2s+1}P_{2s+1}(\varphi)-\sum_{s=n+1}^{M}\zeta(2s+1-2n)\left(i\frac{\chi_0}{K}\right)^{2s+1}P_{2s+1}(\varphi)\,.$$

For the equation (A7), the same method gives

$$\left\{\left\{S_0^Y+\frac{2}{\pi}\left[\ln\left(\frac{k}{2K}\right)+\gamma\right]\right\}\binom{2N}{N}+2\sum_{\ell=1}^{N}\left[S_{2\ell}^Y-\frac{2}{\pi}\frac{(-1)^{\ell}}{\ell}\right](-1)^{\ell}\binom{2N}{N-\ell}\right\}\left(\frac{k}{2}\right)^{2N}$$

$$=-\frac{2}{d}\left\{\sum_{n=n_1+1}^{\infty}\alpha_n^{2N}\left[\frac{1}{\sqrt{\alpha_n^2-k^2}}-\frac{1}{nK}\sum_{s=0}^{2M}\left(i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right]\right.$$
$$\left.+\sum_{n=n_2+1}^{\infty}\alpha_{-n}^{2N}\left[\frac{1}{\sqrt{\alpha_{-n}^2-k^2}}-\frac{1}{nK}\sum_{s=0}^{2M}\left(-i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right]\right\}$$
$$+\frac{1}{\pi}\left\{\sum_{n=1}^{n_1}\frac{\alpha_n^{2N}}{n}\sum_{s=0}^{2M}\left(i\frac{\chi_0}{nK}\right)^s P_s(\varphi)+\sum_{n=1}^{n_2}\frac{\alpha_{-n}^{2N}}{n}\sum_{s=0}^{2M}\left(-i\frac{\chi_0}{nK}\right)^s P_s(\varphi)\right\}$$
$$-\frac{2\alpha_0^{2N}}{\pi}\left\{\sum_{n=0}^{2N}\binom{2N}{n}\left(i\frac{\chi_0}{\alpha_0}\right)^n P_n(\varphi)g(n)-\sum_{n=0}^{N}\binom{2N}{2n}\left(\frac{K}{\alpha_0}\right)^{2n}F_n-\sum_{n=0}^{N-1}\binom{2N}{2n+1}\left(\frac{K}{\alpha_0}\right)^{2n+1}G_n\right\}. \qquad \text{(A14)}$$

To obtain this recurrence relation we have used the relation

$$\sum_{n=0}^{2N}\binom{2N}{n}\left(-\frac{1}{\varphi}\right)^n P_n(\varphi)=\frac{(2N)!}{(N!)^2}\left(\frac{k}{2\alpha_0}\right)^{2N}. \qquad \text{(A15)}$$

The relations (A12) and (A15) are particular cases of the general formula (verified analytically in MATHEMATICA):

$$\sum_{n=0}^{N}\binom{N}{n}\left(-\frac{1}{z}\right)^n P_n(z)=(-1)^{N/2}P_N(0)\left(1-z^2\right)^{N/2}.$$

APPENDIX B: FORMULAS FOR COMPUTATION OF TRANSCENDENTAL FUNCTIONS

The generalized Clausen function is defined as [14]

$$\begin{aligned} \mathrm{Cl}_{2s+1}(\theta) &= \sum_{n=1}^{\infty} \frac{\cos(n\theta)}{n^{2s+1}} \\ &= \mathrm{Re}\left[\mathrm{Li}_{2s+1}(e^{i\theta})\right] , \\ \mathrm{Cl}_{2s+2}(\theta) &= \sum_{n=1}^{\infty} \frac{\sin(n\theta)}{n^{2s+2}} \\ &= \mathrm{Im}\left[\mathrm{Li}_{2s+2}(e^{i\theta})\right] , \ s = 0,1,2,\dots , \end{aligned}$$

where Li represents the polylogarithm function. Their series expansions may be obtained from the relation between the Lerch function $\Phi(z,s,v)$ and the polylogarithm function [15]:

$$z\,\Phi(z,s,1) = \mathrm{Li}_s(z) ,$$

so that

$$\begin{aligned} \mathrm{Cl}_{2s+1}(\theta) &= \mathrm{Re}\left[e^{i\theta}\ \Phi(e^{i\theta}, 2s+1, 1)\right] , \\ \mathrm{Cl}_{2s+2}(\theta) &= \mathrm{Im}\left[e^{i\theta}\ \Phi(e^{i\theta}, 2s+2, 1)\right] . \end{aligned}$$

For $|\ln z| < 2\pi$, $s = 2,3,4\dots$, and $v \neq 0,-1,-2,\dots$, the Lerch function has the series expansion [15]:

$$\begin{aligned} z^v\,\Phi(z,s,v) = & \sum_{n=0}^{\infty}{}' \zeta(s-n,v)\,\frac{(\ln z)^n}{n!} \\ & + \frac{(\ln z)^{s-1}}{(s-1)!}\left[\psi(s) - \psi(v) - \ln(\ln 1/z)\right] . \end{aligned} \tag{B1}$$

Here, $\zeta(s,v)$ is the generalized Riemann ζ function and, the prime indicates that the term with $n = s-1$ is to be omitted.

Substituting in (B1), $z = \exp(i\theta)$ and $\zeta(-n) = -B_{n+1}/(n+1)$, $[\zeta(0) = B_1]$, we obtain

$$\begin{aligned} \mathrm{Cl}_{2s+1}(\theta) = & \sum_{n=0}^{s-1} \frac{\zeta(2s+1-2n)}{(2n)!}(-1)^n\theta^{2n} + \frac{(-1)^s}{(2s)!}g(2s)\ \theta^{2s} - (-1)^s\frac{\theta^{2s}}{(2s)!}\ln|\theta| \\ & - \sum_{n=s+1}^{\infty} B_{2n-2s}(-1)^n\frac{\theta^{2n}}{(2n)!(2n-2s)} , \end{aligned} \tag{B2}$$

$$\begin{aligned} \mathrm{Cl}_{2s+2}(\theta) = & \sum_{n=0}^{s-1} \frac{\zeta(2s+1-2n)}{(2n+1)!}(-1)^n\theta^{2n+1} + \frac{(-1)^s}{(2s+1)!}g(2s+1)\ \theta^{2s+1} - (-1)^s\frac{\theta^{2s+1}}{(2s+1)!}\ln|\theta| \\ & - \sum_{n=s+1}^{\infty} B_{2n-2s}(-1)^n\frac{\theta^{2n+1}}{(2n+1)!(2n-2s)} , \end{aligned} \tag{B3}$$

where $g(s) = \sum_{p=1}^{s} 1/p = \psi(s+1) - \psi(1)$, B_n are the Bernoulli numbers and $\psi(s)$ represents the digamma function.

We mention that, for $0 < \theta < 2\pi$, we also have

$$\mathrm{Cl}_1(\theta) = -\ln|\theta| - \sum_{n=1}^{\infty} B_{2n}(-1)^n\frac{\theta^{2n}}{(2n)!(2n)} .$$

APPENDIX C: LATTICE SUM IDENTITIES

To express the lattice sums (14) and (15) in terms of the lattice sums (7), we apply Neumann's addition theorem for the Hankel functions [13]:

$$H_\ell^{(1)}(k|nd + d/2|) = \sum_{n=-\infty}^{\infty} H_{\ell-m}^{(1)}(|n|kd)J_m(kd/2), \tag{C1}$$

$$H_\ell^{(1)}(k|nd - d/2|) = \sum_{n=-\infty}^{\infty} H_{\ell+m}^{(1)}(|n|kd)J_m(kd/2). \tag{C2}$$

From (14) we obtain

$$\begin{aligned} s_\ell^+ &= (-1)^\ell H_\ell^{(1)}(kd/2) + \sum_{n=1}^{\infty} H_\ell^{(1)}(k|nd - d/2|)\,e^{i\alpha_0 nd} + \sum_{n=1}^{\infty} H_\ell^{(1)}(k|nd + d/2|)\,e^{i\ell\pi}\,e^{-i\alpha_0 nd} \\ &= (-1)^\ell H_\ell^{(1)}(kd/2) + \sum_{n=1}^{\infty}\sum_{m=-\infty}^{\infty} H_{\ell+m}^{(1)}(nkd)J_m(kd/2)e^{i\alpha_0 nd} + \sum_{n=1}^{\infty}\sum_{m=-\infty}^{\infty} H_{\ell-m}^{(1)}(nkd)J_m(kd/2)(-1)^\ell e^{-i\alpha_0 nd} \\ &= (-1)^\ell H_\ell^{(1)}(kd/2) + \sum_{m=-\infty}^{\infty} J_m(kd/2)\sum_{n=1}^{\infty} H_{\ell+m}^{(1)}\left[e^{i\alpha_0 nd} + (-1)^\ell e^{-i\alpha_0 nd}\right] , \end{aligned}$$

and a similar expression for s_ℓ^-. Finally, substituting (8), we get

$$s_\ell^+ = (-1)^\ell H_\ell^{(1)}(kd/2) + \sum_{m=-\infty}^{\infty} S_{\ell+m} J_m(kd/2)\,, \quad \text{(C3)}$$

$$s_\ell^- = H_\ell^{(1)}(kd/2) + \sum_{m=-\infty}^{\infty} S_{\ell-m} J_m(kd/2)\,. \quad \text{(C4)}$$

By means of (16) we obtain the relation

$$\left[e^{i\alpha_0 d} - (-1)^\ell\right] H_\ell^{(1)}(kd/2) = \sum_{m=-\infty}^{\infty} \left[S_{\ell+m} - e^{i\alpha_0 d} S_{\ell-m}\right] J_m(kd/2)\,, \quad \text{(C5)}$$

and, by changing the summation index, we are led to the lattice sum identity:

$$\left[e^{i\alpha_0 d} - (-1)^\ell\right] H_\ell^{(1)}(kd/2) = \sum_{m=-\infty}^{\infty} \left[J_{m-\ell}(kd/2) - e^{i\alpha_0 d} J_{\ell-m}(kd/2)\right] S_m\,, \quad \text{(C6)}$$

or

$$\left[e^{i\alpha_0 d} - (-1)^\ell\right] H_\ell^{(1)}(kd/2) = \sum_{m=-\infty}^{\infty} \left[(-1)^{\ell+m} - e^{i\alpha_0 d}\right] J_{\ell-m}(kd/2) S_m\,. \quad \text{(C7)}$$

To obtain the lattice sum identities for S_ℓ^J and S_ℓ^Y, separately, we rewrite (C7) in the form

$$\left[e^{i\alpha_0 d} - (-1)^\ell\right] H_\ell^{(1)}(kd/2) = \left[(-1)^\ell - e^{i\alpha_0 d}\right] J_\ell(kd/2) S_0 + \sum_{m=1}^{\infty} \left[(-1)^{\ell+m} - e^{i\alpha_0 d}\right] J_{\ell-m}(kd/2) S_m + \sum_{m=1}^{\infty} \left[(-1)^{\ell+m} - e^{i\alpha_0 d}\right] J_{\ell+m}(kd/2) S_{-m}\,.$$

Taking into account that $S_{-m} = (-1)^m S_m$, we have

$$\left[e^{i\alpha_0 d} - (-1)^\ell\right] \left[H_\ell^{(1)}(kd/2) + S_0 J_\ell(kd/2)\right] = \sum_{m=1}^{\infty} \left[(-1)^{\ell+m} - e^{i\alpha_0 d}\right] \times \left[J_{\ell-m}(kd/2) + (-1)^m J_{\ell+m}(kd/2)\right] S_m\,.$$

Now, we split the series in the right hand side, for lattice sums of even and odd order:

$$\left[e^{i\alpha_0 d} - (-1)^\ell\right]\left[H_\ell^{(1)}(kd/2) + S_0 J_\ell(kd/2)\right] = \sum_{m=1}^{\infty} \left[(-1)^\ell - e^{i\alpha_0 d}\right] \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m} - \sum_{m=1}^{\infty} \left[(-1)^\ell + e^{i\alpha_0 d}\right] \times \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1}\,. \quad \text{(C8)}$$

From (9) and (10), we deduce the relations:

$$S_{2\ell}(-\alpha_0, k, d) = S_{2\ell}(\alpha_0, k, d)\,, \quad \text{(C9)}$$

$$S_{2\ell-1}(-\alpha_0, k, d) = -S_{2\ell-1}(\alpha_0, k, d)\,. \quad \text{(C10)}$$

so that we have two relations of the form (C8)

$$\left[e^{i\alpha_0 d} - (-1)^\ell\right] \left\{ H_\ell^{(1)}(kd/2) + S_0 J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m} \right\} + \left[e^{i\alpha_0 d} + (-1)^\ell\right] \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1} \right\} = 0\,,$$

for α_0, and

$$\left[e^{-i\alpha_0 d} - (-1)^\ell\right] \left\{ H_\ell^{(1)}(kd/2) + S_0 J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m} \right\} - \left[e^{-i\alpha_0 d} + (-1)^\ell\right] \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1} \right\} = 0\,,$$

for $-\alpha_0$. The sum and difference of these two equations give us

$$\left[\cos(\alpha_0 d) - (-1)^\ell\right] \left\{ H_\ell^{(1)}(kd/2) + S_0 J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m} \right\}$$
$$+ i \sin(\alpha_0 d) \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1} \right\} = 0\,, \quad \text{(C11)}$$

$$i \sin(\alpha_0 d) \left\{ H_\ell^{(1)}(kd/2) + S_0 J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m} \right\}$$
$$+ \left[\cos(\alpha_0 d) + (-1)^\ell\right] \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1} \right\} = 0\,. \quad \text{(C12)}$$

Now, we may use (9) and (10) to split these equations into the real and imaginary parts. Consequently, we have

$$\left[\cos(\alpha_0 d) - (-1)^\ell\right] \left\{ J_\ell(kd/2) + S_0^J J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m}^J \right\}$$
$$- \sin(\alpha_0 d) \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1}^J \right\} = 0\,, \quad \text{(C13)}$$

$$\sin(\alpha_0 d) \left\{ J_\ell(kd/2) + S_0^J J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m}^J \right\}$$
$$+ \left[\cos(\alpha_0 d) + (-1)^\ell\right] \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1}^J \right\} = 0\,, \quad \text{(C14)}$$

for S_m^J, and

$$\left[\cos(\alpha_0 d) - (-1)^\ell\right] \left\{ Y_\ell(kd/2) + S_0^Y J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m}^Y \right\}$$
$$- \sin(\alpha_0 d) \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1}^Y \right\} = 0\,, \quad \text{(C15)}$$

$$\sin(\alpha_0 d) \left\{ Y_\ell(kd/2) + S_0^Y J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m}^Y \right\}$$
$$+ \left[\cos(\alpha_0 d) + (-1)^\ell\right] \left\{ \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1}^Y \right\} = 0\,, \quad \text{(C16)}$$

for S_m^Y.

Not all these equations are independent. If we denote by

$$A_\ell = \left(1 + S_0^J\right) J_\ell(kd/2) + \sum_{m=1}^{\infty} \left[J_{\ell-2m}(kd/2) + J_{\ell+2m}(kd/2)\right] S_{2m}^J\,, \tag{C17}$$

$$B_\ell = \sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(kd/2) - J_{\ell+2m-1}(kd/2)\right] S_{2m-1}^J\,, \tag{C18}$$

in (C13) and (C14), we obtain the homogeneous system:

$$A_\ell \left[\cos(\alpha_0 d) - (-1)^\ell\right] - B_\ell \sin(\alpha_0 d) = 0,$$
$$A_\ell \sin(\alpha_0 d) + B_\ell \left[\cos(\alpha_0 d) + (-1)^\ell\right] = 0\,,$$

whose determinant vanishes identically for all $\ell \in \mathcal{Z}$. The same remark also applies to (C15) and (C16).

The first equation, (C13), is identically satisfied by the expressions (A9) and (A10). To prove this, we make use of the relation [16]:

$$\sum_{k=-\infty}^{\infty} \left\{ \begin{array}{c} \sin(k\alpha) \\ \cos(k\alpha) \end{array} \right\} J_{k+n}(z) = \left\{ \begin{array}{c} \sin(-n\alpha + z\sin\alpha) \\ \cos(n\alpha - z\sin\alpha) \end{array} \right\}, \tag{C19}$$

where z and α are independent variables. Taking into account that, for integer orders, the Bessel functions satisfy the relation $J_\ell(-z) = (-1)^\ell J_\ell(z)$, and combining relations of the form (C19), for z and $-z$, we obtain the following equations:

$$\sum_{m=1}^{\infty} \left[J_{\ell-2m}(z) + J_{\ell+2m}(z)\right] \cos(2m\alpha) = -J_\ell(z) + \left\{ \begin{array}{ll} \cos(\ell\alpha)\cos(z\sin\alpha) & ;\ell = \text{even} \\ -\sin(\ell\alpha)\sin(z\sin\alpha) & ;\ell = \text{odd} \end{array} \right\} \tag{C20}$$

and

$$\sum_{m=1}^{\infty} \left[J_{\ell-2m+1}(z) - J_{\ell+2m-1}(z)\right] \sin[(2m-1)\alpha] = (-1)^{\ell+1} \sum_{m=-\infty}^{\infty} J_{2m-1-\ell}(z) \sin[(2m-1)\alpha] = \left\{ \begin{array}{ll} -\cos(\ell\alpha)\sin(z\sin\alpha) & ;\ell = \text{even} \\ -\sin(\ell\alpha)\cos(z\sin\alpha) & ;\ell = \text{odd} \end{array} \right\}. \tag{C21}$$

By substituting (A9) and (A10) into (C17) and (C18), respectively, then using (C20) and (C21) we obtain

$$A_\ell \left[\cos(\alpha_0 d) - (-1)^\ell\right] - B_\ell \sin(\alpha_0 d) \equiv 0\,.$$

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