Efficient Evaluation of Doubly Periodic Green Functions in 3D Scattering, Including Wood Anomaly Frequencies

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Abstract

We present efficient methods for computing wave scattering by diffraction gratings that exhibit two-dimensional periodicity in three dimensional (3D) space. Applications include scattering in acoustics, electromagnetics and elasticity. Our approach uses boundary-integral equations. The quasi-periodic Green function employed is structured as a doubly infinite sum of scaled 3D free-space outgoing Helmholtz Green functions. Their source points are located at the nodes of a periodicity lattice of the grating; the scaling is effected by Bloch quasi-periodic coefficients.

For efficient numerical computation of the lattice sum, we employ a smooth truncation. Super-algebraic convergence to the Green function is achieved as the truncation radius increases, except at frequency-wavenumber pairs at which a Rayleigh wave is at exactly grazing incidence to the grating. At these "Wood frequencies", the term in the Fourier series representation of the Green function that corresponds to the grazing Rayleigh wave acquires an infinite coefficient and the lattice sum blows up. A related challenge occurs at non-exact grazing incidence of a Rayleigh wave; in this case, the constants in the truncation-error bound become too large.

At Wood frequencies, we modify the Green function by adding two types of terms to it. The first type adds weighted spatial shifts of the Green function to itself. The shifts are such that the spatial singularities introduced by these terms are located below the grating and therefore out of the domain of interest. With suitable choices of the weights, these terms annihilate the growing contributions in the original lattice sum and yield algebraic convergence. The degree of the algebraic convergence depends on the number of the added shifts. The second-type terms are quasi-periodic plane wave solutions of the Helmholtz equation. They reinstate (with controlled coefficients now) the grazing modes, effectively eliminated by the terms of first type. These modes are needed in the Green function for guaranteeing the well-posedness of the boundary-integral equation that yields the scattered field.

We apply this approach to acoustic scattering by a doubly periodic 2D grating near and at Wood frequencies and scattering by a doubly periodic array of scatterers away from Wood frequencies.

This manuscript is a preliminary version of our work, which is made available through arXiv to facilitate rapid dissemination. A more developed text is in preparation.

Keywords: scattering, periodic Green function, lattice sum, smooth truncation, Wood frequency, Wood anomaly, boundary-integral equations, electromagnetic computation

1 Introduction

Calculation of wave scattering by doubly periodic structures in electromagnetics, acoustics, and elasticity poses serious computational challenges. Such structures include a planar grating or a material slab whose geometry is repeated periodically in two directions and is of finite extent in the third. As is well known from Bloch theory, a periodic geometry gives rise to quasi-periodic fields. The Green function for the Helmholtz equation $\Delta u + k^2 u = 0$ in three dimensions that has two-dimensional quasi-periodicity is ubiquitous in these calculations, whether they involve scalar or vector fields. It is put together as an infinite sum of three-dimensional, free-space, outgoing Helmholtz Green functions. Their singularities are placed at the points of the planar lattice of periodicity and they are scaled by Bloch quasi-periodic coefficients,

$$G_k^{qper}(\mathbf{x}) \;=\; \frac{1}{4\pi}\sum_{m,n\in\mathbb{Z}} \frac{e^{ikr_{mn}}}{r_{mn}} e^{-i(\alpha m d_1 + \beta n d_2)}. \tag{1}$$

In this formula[1], $\mathbf{x} = (x, y, z)$ is the spatial coordinate, the vector (d_1, d_2) defines the period cell, (α, β) is the Bloch wave-vector and $r_{mn}^2 = (x + md_1)^2 + (y + nd_2)^2 + z^2$.

Another representation of the Green function is obtained by applying the Poisson summation formula to the series (1) and will also be of use to us. It is an expansion in Rayleigh waves[2] with the summation over the dual lattice,

$$G_k^{qper}(\mathbf{x}) = \frac{i}{2d_1 d_2}\sum_{j,\ell\in\mathbb{Z}} \frac{1}{\gamma_{j\ell}} e^{i(\alpha_j x + \beta_\ell y)} e^{i\gamma_{j\ell}|z|}\,, \tag{2}$$

where

$$\alpha_j = \alpha + \frac{2\pi j}{d_1},\;\; \beta_\ell = \beta + \frac{2\pi \ell}{d_2},\;\; \gamma_{j\ell} = (k^2 - \alpha_j^2 - \beta_\ell^2)^{\frac{1}{2}}. \tag{3}$$

In the determination of the square root that defines $\gamma_{j\ell}$, positive numbers have positive square root and the branchcut is the negative imaginary semiaxis. Rayleigh waves then either decay as $|z|$ increases (evanescent modes) or are outgoing traveling waves (propagating modes). There are at most finitely many propagating modes. Rayleigh waves for which $\gamma_{j\ell}$ is small are of "grazing incidence" to the periodic structure; they dominate the sum (2) and tend to the z-independent, exactly grazing, waves $e^{i(\alpha_j x + \beta_\ell y)}$ as $\gamma_{j\ell} \to 0$.

As is well known, and as it was first noticed by Wood [15] and first explained mathematically by Rayleigh [16], a certain type of anomalous scattering behavior, the "Wood anomaly", is associated with a grazing mode, that is, one for which the coefficient $\gamma_{j\ell}$ vanishes. Parameter values, such as frequencies, wavenumbers, periods etc., for which this coefficient equals zero are often referred to as Wood anomaly values of the parameters. Assuming, as often happens, that all parameters except one, *e.g.* the frequency (resp. incidence angle, etc.) are held fixed, "Wood anomaly frequencies" (resp. Wood anomaly incidence angles, etc.) are those frequencies (resp. incidence angles, etc.) for which one of the coefficients $\gamma_{j\ell}$ is equal to zero. For convenience, one sometimes says that a Wood anomaly occurs at that particular value of the parameter. Wood anomaly frequencies are also called "cutoff frequencies", since the corresponding Rayleigh mode, or diffraction order, switches from propagating to evanescent. We refer to them usually as "Wood frequencies".

The major contribution of the present work is a method of efficient and accurate evaluation of wave scattering by 2D periodic structures at Wood frequencies. The corresponding problem concerning 1D periodic structures in 2D is treated in [3]. These contributions were announced in [7] and [4].

The poor convergence properties of the lattice sum (1), which are notorius even away from Wood anomalies, have been extensively discussed in the literature, and various methods to accelerate its

[1](1) is the Floquet transform of the free-space radiating Green function $e^{ikr}/(4\pi r)$ for the Helmholtz equation.

[2]exponential solutions of Helmholtz equation commensurate with the Bloch wavevector

convergence, notably the Ewald method [10, 8], have been proposed. A survey is given in [12]. The challenge in the calculation of the Green function is two-fold.

1. The lattice sum does not converge absolutely. At all frequencies, except Wood frequencies, it does converge conditionally [6], but its convergence rate of $\sim C/r$ is too slow to be computationally feasible.

2. At a Wood frequency, when $\gamma_{j\ell}$ vanishes for some (j,ℓ) (exact grazing), the lattice sum (1) does not converge at all and a coefficient in the Rayleigh-wave expansion (2) becomes infinite. In fact, in this case the quasi-periodic Green function does not exist. At frequencies near a Wood frequency, at least one $\gamma_{j\ell}$ is small and the corresponding coefficient in (2) is large. This translates to even slower convergence in (1).

We address both of these challenges in the present work. We use a smooth truncation of the lattice sum (1), that obtains super-algebraic convergence to the radiating quasi-periodic Green function as the radius of truncation increases, as long as one is not at a Wood frequency. Near and at Wood frequencies, the truncation, supplemented with a modification of the lattice sum, produces rapid algebraic convergence to an altered Green function. The modification is inspired by the classic method of images and consists of adding weighted, shifted copies of each term of the sum to itself. The source points of the shifted terms are placed outside the domain of implementation of the Green function, thus these terms supplement the original term with a smooth field. The impact of the modification is to supress lattice sum contributions that effectively add up to grazing modes. Such modes are supressed entirely at Wood frequencies and almost entirely near them, resulting in the improved convergence.

Our approach uses boundary-integral equations (see section 2). The supression of the grazing modes, while producing the desired efficient convergence and computation of the Green function, compromises the numerical stability (at Wood frequencies even the well-posedness) of the boundary-integral formulation. This defect is countered by making the additional simple modification to the Green function of explicitly adding back the grazing Rayleigh waves with appropriately sized coefficients. For problems of scattering by 1D-periodic structures in 2D space, computation of the quasi-periodic Green function can be avoided [1] by employing auxiliary layer potentials on the 1D boundary of the unit cell.

We demonstrate efficient and accurate computation of the Green functions with problems of scattering of time-harmonic scalar acoustic plane waves in section 6. For non-Wood frequencies, we compute scattering by a periodic array of obstacles, defined through $\Omega_{per} = \cup_{(m,n)\in\mathbb{Z}\times\mathbb{Z}}\Omega_{m,n}$, where $\Omega_{0,0} = \Omega$ is a bounded region in $\mathbb{R}^3$ whose boundary S is a closed or open surface, $\Omega_{m,n}$ are the shifts $\Omega_{m,n} = \Omega + md_1\mathbf{e}_1 + nd_2\mathbf{e}_2$ in terms of the standard vectors $\mathbf{e}_1$ and $\mathbf{e}_2$, and the periods d_1 and d_2 chosen to be larger than the diameter of Ω.

At and near Wood frequencies, we compute scattering by a periodic grating— an infinite surface with doubly periodic geometry, which is represented as the graph in $\mathbb{R}^3$ of a function that has periods d_1 and d_2,

$$z = f(x,y), \qquad f(x+d_1, y+d_2) = f(x,y)\,. \tag{4}$$

In the case of a periodic array of obstacles, define the regions above and below the array by $\Omega_+ = \{\mathbf{x} : z > \max z', (x',y',z') \in \Omega_{per}\}$, and $\Omega_- = \{\mathbf{x} : z < \min z', (x',y',z') \in \Omega_{per}\}$. We will consider the sound-soft scattering problem

$$\begin{aligned} \Delta u + k^2 u &= 0 \text{ in } \mathbb{R}^3 \setminus \Omega_{per} \\ u &= -u^{inc} \text{ on } \partial\Omega_{per} \end{aligned} \tag{5}$$

where the incident field is taken to be a plane wave from above with propagation vector $(\alpha, \beta, -\gamma)$,

$$u^{inc}(\mathbf{x}) = \exp(ik\mathbf{d} \cdot \mathbf{x}) = \exp[i(\alpha x + \beta y - \gamma z)] \tag{6}$$

given in spherical coordinates by the relations $\alpha = k \sin\psi \cos\phi$, $\beta = k \sin\psi \sin\phi$, and $\gamma = k \cos\psi$. In order to retrieve the physically realizable solutions of the scattering problem, one must supplement equations (5) with radiations conditions on the fields u in the regions Ω_+ and Ω_-. The radiations conditions can be expressed via the classical Raleigh series owing to the periodicity of the domain Ω_{per} and the form of the incident field. Specifically, denoting by u^+ and u^- the scattered fields in the regions Ω_+ and Ω_-, one has

$$\begin{aligned} u^+(\mathbf{x}) &= \sum_{j,\ell \in \mathbb{Z}} B^+_{j\ell} \exp[i(\alpha_j x_1 + \beta_\ell x_2 + \gamma_{j\ell} x_3)], \ \mathbf{x} \in \Omega_+ & (7) \\ u^-(\mathbf{x}) &= \sum_{j,\ell \in \mathbb{Z}} B^-_{j\ell} \exp[i(\alpha_j x_1 + \beta_\ell x_2 - \gamma_{j\ell} x_3)], \ \mathbf{x} \in \Omega_-. & (8) \end{aligned}$$

Applications of our method to penetrable scatterers and to vector equations as in electromagnetics will be treated in further communications.

In the case of time-harmonic scattering problems from doubly periodic surfaces, we let $\Gamma = \{(x, y, z) : z = f(x, y)\}$, $\Gamma_+ = \{(x, y, z) : z > f(x, y)\}$, and $\Gamma_- = \{(x, y, z) : z < f(x, y)\}$. We will consider total reflection of a plane wave incident on the surface Γ from above. In the absence of transmission, the region below the surface, labeled Γ_-, is outside the domain of interest. In acoustic scattering, the "sound-soft" acoustic case requires the Dirichlet boundary condition and the "sound-hard" case requires the Neumann condition,

$$\begin{aligned} \Delta u + k^2 u &= 0 \text{ in } \Gamma^+ & \\ u &= -u^{inc} \text{ on } \Gamma \quad \text{(sound-soft)} & (9) \\ \frac{\partial u}{\partial \mathbf{n}} &= -\frac{\partial u^{inc}}{\partial \mathbf{n}} \text{ on } \Gamma \quad \text{(sound-hard).} & (10) \end{aligned}$$

The scattered field for $z > \max f$ satisfies a radiation condition on the modes of the classical Rayleigh series,

$$u^+(\mathbf{x}) = \sum_{j,\ell \in \mathbb{Z}} B^+_{j\ell} \exp[i(\alpha_j x_1 + \beta_\ell x_2 + \gamma_{j\ell} x_3)], \quad z > \max f. \tag{11}$$

The sound-soft scattering problem has a unique solution [14].

We conclude the introduction with a summary of the main results in this study and reference to the corresponding theorems in the text.

1. **Away from Wood frequencies.** Multiplying the infinite lattice sum (1) by a smooth truncation function $\chi(md_1/a, nd_2/a)$, we obtain a finite sum that converges super-algebraically to the infinite sum as $a \to \infty$ (Theorem 3.1). The truncation function χ equals unity when (m, n) is within a certain radius and equals zero when it lies outside of a larger radius. It varies smoothly in the annulus between the two radii. The radii increase linearly with the truncation radius a. The proof is based on the Poisson summation formula. A continuous version of this result is proved in [13] for smooth diffraction gratings in $\mathbb{R}^2$.

2. **At or near Wood frequencies.** At Wood frequencies, the lattice sum (1) does not converge; the corresponding term in the Fourier series representation of the Green function (2) acquires an infinite coefficient ($\gamma_{j\ell} = 0$). At nearly Wood frequencies, one or more of the $\gamma_{j\ell}$ are small and nonzero, the super-algebraic convergence slows down and the constants in the algebraic error estimates grow large. In both cases, we modify the Green function by adding two types of terms to it.

   - The first type adds to the Green function weighted copies of itself, in which the sources have been shifted in the negative z direction. Since the source points in the boundary-integral formulation are on the surface Γ, shifting them in this way moves them *below* the surface and thus out of the domain of interest. With suitable choice of the weights, the introduced terms supress the growing contributions in the original lattice sum, as discussed above, and produce algebraic convergence in the truncation process. The Green function, modified by the addition of the terms of the first type is given by

$$G_k^{qper,p}(\mathbf{x}) = \frac{1}{4\pi} \sum_{m,n\in\mathbb{Z}} e^{-i(\alpha m d_1 + \beta n d_2)} \sum_{q=0}^{p} a^{pq} \frac{e^{ikr_{mn}^{pq}}}{r_{mn}^{pq}} , \tag{12}$$

     in which $r_{mn}^{pq} = \sqrt{(x+md_1)^2 + (y+nd_2)^2 + (z+qd)^2}$. The term corresponding to $a_{p0} = 1$ represents the unmodified Green function. The degree of the algebraic convergence depends on the number of the added shifts. We obtain algebraic convergence like C/a^{ν}, where $\nu = \lceil p/2 \rceil - 1/2$, as the truncation radius a grows (Theorem 4.3).

   - The second type terms added to the Green function are quasi-periodic plane-wave solutions of the Helmholtz equation. They re-instate (with controlled coefficients now) the grazing modes, effectively eliminated by the terms of first type. These modes are needed in the Green function for guaranteeing the well-posedness of the boundary-integral equation (it uses a combined single- and double-layer potential) that yields the unique solution for acoustic reflection off a periodic grating (Theorem 4.1). The corresponding problem concerning 1D periodic structures in 2D is treated in [3]. These contributions were announced in [7] and [4].

3. **Numerical computations.** Section 5 describes the numerical method used to implement the fast lattice sums and compute the densities in the boundary-integral representation of the scattered field. Section 6 shows numerical results at and away from Wood frequencies.

This manuscript is a preliminary version of our work on computation of doubly periodic Green functions in three dimensions, which is made available through arXiv to facilitate rapid dissemination. A more developed text is in preparation.

2 Integral equations for periodic scattering problems

In the case when Ω is a closed surface, we look for scattered fields u which are solutions of equations (5) in the form of a combined field layer potential

$$u(\mathbf{x}) = \int_{S_{per}} \frac{\partial G_k(|\mathbf{x}-\mathbf{x}'|)}{\partial \mathbf{n}(\mathbf{x}')} \mu_{per}(\mathbf{x}') ds(\mathbf{x}') + i\tau \int_{S_{per}} G_k(|\mathbf{x}-\mathbf{x}'|) \mu_{per}(\mathbf{x}') ds(\mathbf{x}') \tag{13}$$

in terms of the unknown surface density μ_{per} and the outgoing free-space Green function $G_k(|\mathbf{z}|) = \frac{e^{ik|\mathbf{z}|}}{4\pi|\mathbf{z}|}$. The coupling constant τ is real, and $\mathbf{n}$ is the unit normal to the surface S_{per} pointing in the exterior of the domain Ω_{per}. Using the jump properties of the layer potentials and the sound soft boundary conditions, the unknown density μ_{per} is a solution of the combined field integral equation

$$\begin{aligned}\frac{\mu_{per}(\mathbf{x})}{2} + \int_{S_{per}} \frac{\partial G_k(|\mathbf{x}-\mathbf{x}'|)}{\partial \mathbf{n}(\mathbf{x}')}\mu_{per}(\mathbf{x}')ds(\mathbf{x}') \quad &+ \quad i\tau \int_{S_{per}} G_k(|\mathbf{x}-\mathbf{x}'|)\mu_{per}(\mathbf{x}')ds(\mathbf{x}') \\ &= \quad -\exp(ik\mathbf{d}\cdot\mathbf{x}),\ \mathbf{x}\in S_{per}. \end{aligned} \tag{14}$$

For problems of scattering by doubly periodic surfaces Γ, we seek scattered fields u which are solutions of equations (9) in the form of a combined field

$$u(\mathbf{x}) = \int_\Gamma \left(i\eta G_k(|\mathbf{x}-\mathbf{x}'|) + \xi \frac{\partial G_k(|\mathbf{x}-\mathbf{x}'|)}{\partial \mathbf{n}(\mathbf{x}')} \right) \phi(\mathbf{x}')ds(\mathbf{x}'), \quad \mathbf{x}\in \mathbb{R}^3 \setminus \Gamma \tag{15}$$

in terms of the unknown surface density ϕ, where $\mathbf{n}$ is the unit normal to Γ pointing into Γ_+, and η and ξ are *real* numbers. Using the jump property of the double-layer potentials, the continuity of the single-layer potentials, and the sound-soft (Dirichlet) boundary condition, the unknown density ϕ is a solution of the integral equation

$$\frac{\xi\phi(\mathbf{x})}{2} + \int_\Gamma \left(i\eta G_k(|\mathbf{x}-\mathbf{x}'|) + \xi \frac{\partial G_k(|\mathbf{x}-\mathbf{x}'|)}{\partial \mathbf{n}(\mathbf{x}')} \right) \phi(\mathbf{x}')ds(\mathbf{x}') = -e^{ik\mathbf{d}\cdot\mathbf{x}},\ \mathbf{x}\in\Gamma. \tag{16}$$

Equations (14) and (16) can be rewritten in a form that involves integration *only over one period cell*, that is the surface S in the former case and the scattering surface $\Gamma^{per} = \{(x,y,z) : 0 \le x < d_1,\ 0 \le y < d_2,\ z = f(x,y)\}$ in the latter case. Away from Wood frequencies, this is done with the aid of the (α,β) quasi-periodic Green function (1), in which $\mathbf{x}$ is replaced by the difference between source and influence points,

$$G_k^{qper}(\mathbf{x}-\mathbf{x}') = \sum_{m,n=-\infty}^{\infty} G_k(x-x'+md_1, y-y'+nd_2, z-z')e^{-i\alpha m d_1}e^{-i\beta n d_2}. \tag{17}$$

At or near Wood frequencies, and in the case of scattering problems off doubly periodic surfaces, we use a modified Green function, as explained above.

The densities μ and ϕ respectively are now defined on the period cells S and Γ^{per} where they satisfy quasi-periodic (Bloch) conditions. The integral equation formulations for the sound-soft case can be written in the form

$$\begin{aligned}\frac{\mu(\mathbf{x})}{2} + \int_S \frac{\partial G_k^{per}(\mathbf{x},\mathbf{x}')}{\partial \mathbf{n}(\mathbf{x}')}\mu(\mathbf{x}')ds(\mathbf{x}') \quad &+ \quad i\tau \int_S G_k^{per}(\mathbf{x},\mathbf{x}')\mu(\mathbf{x}')ds(\mathbf{x}') \\ &= \quad -\exp(ik\mathbf{d}\cdot\mathbf{x}),\ \mathbf{x}\in S. \end{aligned} \tag{18}$$

and

$$\begin{aligned}\frac{\xi\phi(\mathbf{x})}{2} \quad &+ \quad \int_{\Gamma^{per}} \left(i\eta G_k^{qper}(\mathbf{x},\mathbf{x}') + \xi \frac{\partial G_k^{qper}(\mathbf{x},\mathbf{x}')}{\partial \mathbf{n}(\mathbf{x}')} \right) \phi(\mathbf{x}')ds(\mathbf{x}') \\ &= \quad -e^{ik(d_1x+d_2y+d_3f(x,y))},\ (x,y),\ (x',y')\in[0,d_1]\times[0,d_2]. \end{aligned} \tag{19}$$

Thus, one must solve Eq. (18) and (19) in order to determine the densities $\mu(\mathbf{x})$ and $\phi(\mathbf{x})$ and insert them into Equations (13) and (15) respectively in order to calculate the corresponding scattered field.

For completeness, we recall that the function $G_k^{qper}(\mathbf{x})$ satisfies

$$G_k^{qper}(\mathbf{x} + (md_1, nd_2, 0)) = G_k^{qper}(\mathbf{x}) e^{i(\alpha m d_1 + \beta n d_2)} \quad \text{for all } m, n \in \mathbb{Z}\,,$$
$$\nabla^2 G_k^{qper}(\mathbf{x}) + k^2\, G_k^{qper}(\mathbf{x}) \;=\; -\sum_{m,n} \delta(x - md_1, y - nd_2, z) e^{i(\alpha m d_1 + \beta n d_2)}\,.$$

Next, we establish sufficient conditions so that the integral equations (19) are uniquely solvable in $L^2([0,d_1] \times [0,d_2])$. In order to prove this we need the following classical result.

Lemma 2.1. *If $u(\mathbf{x})$ is a quasi-periodic field that satisfies the Helmholtz equation $\Delta u + k^2 u = 0$ for $z < f(x,y)$ (resp. $z > f(x,y)$), the outgoing condition (7) (resp. (8)), and the impedance condition on the boundary Γ,*

$$\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}) - i\zeta\, u(\mathbf{x}) = 0 \qquad (\mathbf{x} \in \Gamma)\,,$$

with $\zeta > 0$ (resp. $\zeta < 0$), then $u(\mathbf{x}) = 0$ for $z < f(x,y)$ (resp. $z > f(x,y)$).

Proof. Let u be defined for $z < f(x,y)$ and $\zeta > 0$. The other case is handled analogously. Consider the truncated period

$$\Omega = \{\mathbf{x} : 0 < x < d_1,\ 0 < y < d_2,\ z_- < z < f(x,y)\}$$

with lower boundary $S = \{\mathbf{x} : 0 < x < d_1,\ 0 < y < d_2,\ z = z_-\}$, oriented downward. One computes

$$0 = \int_\Omega (\Delta u + k^2 u)\bar{u} = \int_\Omega \left(-|\nabla u|^2 + k^2 |u|^2\right) dx - \int_\Gamma \frac{\partial u}{\partial n}\, \bar{u}\; ds - \int_S \frac{\partial u}{\partial n}\, \bar{u}\; ds\,. \tag{20}$$

The integration over the lateral sides of Ω vanishes because of the quasi-periodicity of u. The impedance condition on Γ and the outgoing condition (8) give

$$\int_\Gamma \frac{\partial u}{\partial n}\, \bar{u}\; ds \;+\; \int_S \frac{\partial u}{\partial n}\, \bar{u}\; ds \;=\; i\zeta \int_\Gamma |u|^2\; ds \;+\; \frac{i}{2d_1 d_2} \sum_{(j,\ell),\gamma_{j\ell}>0} \gamma_{j\ell} |c_{j\ell}^-|^2$$

This is the imaginary part of (20), and thus $u = 0$ on Γ, and the impedance condition gives $\partial u / \partial \mathbf{n} = 0$ on Γ also. By Holmgren's theorem, $u = 0$ in Ω and therefore for all $\mathbf{x}$ with $z < f(x,y)$. $\square$

The main result about the unique solvability of equations (19) is this:

Theorem 2.2. *Assume that k is a wavenumber such that the quasi-periodic Green function exists, i.e., $\gamma_{j\ell} \neq 0$ for all pairs (j,ℓ). Then the integral equation* (19) *is uniquely solvable in $L^2([0,d_1] \times [0,d_2])$ provided that $\frac{\eta}{\xi} < 0$.*

Proof. Given that the surface Γ is smooth and that G_k^{qper} has the same singularity as G_k, the integral operators in the left-hand side of equation (19) are compact perturbations of a multiple of the identity operator in the space $L^2([0,d_1] \times [0,d_2])$. Thus, by Fredholm theory, the unique solvability of equation (19) is equivalent to the injectivity of the operators featured in the left-hand side of equation (19). Let $\phi_0 \in L^2([0,d_1] \times [0,d_2])$ denote a solution of equation (19) with zero right hand-side, and define by $u^\pm$ the restrictions to $\Gamma^\pm$ of the potential u defined in equation (15) with density ϕ_0. It follows that u^+ is a radiating solution of the Helmholtz equation in Γ^+ with zero Dirichlet boundary conditions, and hence $u^+ = 0$ in Γ^+ [14]. Using the jump relations of scattering boundary-integral operators we obtain that $u^-|_\Gamma = -\xi\phi_0$ and $\left(\frac{\partial u^-}{\partial \mathbf{n}}\right)|_\Gamma = i\eta\phi_0$. Thus ϕ_0 is a radiating solution of the Helmholtz equation in Γ^- with zero impedance boundary conditions $\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}) - i\zeta\, u(\mathbf{x}) = 0,\ \zeta = -\frac{\eta}{\xi} > 0$ on Γ. By Lemma 2.1, $u^- = 0$ in Γ^-, and thus $\phi_0 = 0$ in $L^2([0,d_1]\times[0,d_2])$, which completes the proof of the theorem. □

In the case of Neumann boundary conditions, there are no uniqueness results of the scattering problems, even away from Wood anomalies. Assuming that the wavenumber k is such that the scattering problem described in equations (9,11) has a unique solution, we seek for the scattered field in the form

$$u(\mathbf{x}) = \int_\Gamma G_k(|\mathbf{x}-\mathbf{x}'|)\psi(\mathbf{x}')ds(\mathbf{x}'), \quad \mathbf{x}\in\mathbb{R}^3\setminus\Gamma \tag{21}$$

in terms of the unknown surface density ψ. Using the jump property of the normal derivatives of single-layer potentials and the sound-hard (Neumann) boundary condition, the unknown density ψ is a solution of the integral equation

$$-\frac{\psi(\mathbf{x})}{2} + \int_\Gamma \frac{\partial G_k(|\mathbf{x}-\mathbf{x}'|)}{\partial \mathbf{n}(\mathbf{x})}\psi(\mathbf{x}')ds(\mathbf{x}') = -ik\mathbf{d}\cdot\mathbf{n}(\mathbf{x})\ e^{ik\mathbf{d}\cdot\mathbf{x}},\ \mathbf{x}\in\Gamma. \tag{22}$$

Given that the scattering problems from doubly periodic surfaces and DIrichlet boundary conditions admit unique solutions for all wavenumbers, it follows immediately that the integral equations (22) have themselves unique solutions.

3 Fast convergence of lattice sums by smooth truncation

In this section, we examine the case in which there is no pair of integers (j,ℓ) for which $\gamma_{j\ell} = 0$, that is, the condition

$$k^2 = \left(\alpha + \frac{2\pi j}{d_1}\right)^2 + \left(\beta + \frac{2\pi\ell}{d_2}\right)^2, \quad \text{Wood, or cutoff, condition} \tag{23}$$

is false for all (j,ℓ). In this case, as discussed above, the quasi-periodic Green function exists.

We propose a method for fast evaluation of periodic Green functions by truncating the lattice sum by a smooth truncation function χ with compact support that is equal to unity in a neighborhood of the origin:

$$G_k^{qper}(x,y,z) \;\approx\; G_k^a(x,y,z) := \frac{1}{4\pi}\sum_{m,n\in\mathbb{Z}} \frac{e^{ikr_{mn}}}{r_{mn}} e^{-i(\alpha m d_1 + \beta n d_2)}\,\chi(\tfrac{d_1 m}{a},\tfrac{d_2 n}{a})\,, \tag{24}$$

in which $r_{mn} = ((x+md_1)^2 + (y+nd_2)^2 + z^2)^{\frac{1}{2}}$ and a is a large number. Typically, χ will be either a radial function or one that is separable in x and y,

$$\chi(s,t) \;=\; \psi(\sqrt{s^2+t^2}) \qquad \text{or} \qquad \chi(s,t) \;=\; \psi(s)\psi(t)$$

with $\psi(u)$ being a smooth monotonic function equal to unity for $|u|\le A$ and equal to nullity for $|u|\ge A$ $(0<A<B)$. As a grows, G_k^a converges very fast to G_k^{qper}—in fact, the convergence is faster than any power of a. Theorem 3.1 establishes the super-algebraic convergence of $G_k^a(\mathbf{x})$ on compact sets to a radiating quasi-periodic Green function $G_k^{qper}(\mathbf{x})$ for non-Wood frequencies. The convergence fails at Wood frequencies; in fact, the constants in the convergence rates of the form

C/a^n become unbounded as $\omega = ck$ approaches a Wood frequency. We deal with this issue in section 4.3 by adding a number of reflections of the Green function about the z-axis.

Remark. There is an alternate variation of the method of approximation by a smooth truncation that one could employ instead, namely making the truncation function in (24) dependent on $\mathbf{x}$: $\chi(\frac{x+d_1 m}{a}, \frac{y+d_2 n}{a})$. Boundary-integral computations are performed with $\mathbf{x}$ ranging within a single spatial period, and when a is large, there is negligible difference between the two formulations within this range. One can prove super-algebraic convergence in either case, and there is no real need to analyze both. We find that omitting the dependence on $\mathbf{x}$ is a bit more convenient, so we deal with that case. Nevertheless, it is interesting to compare the two formulations.

The function G_k^a as defined in (24) is simply the Helmholtz field produced by a finite number of radiating monopoles with various weights, situated at points on the lattice $d_1\mathbb{Z} \times d_2\mathbb{Z}$. It satisfies the Helmholtz field but is not quasi-periodic—being a finite sum of monopole-source fields, it decays inversely to the distance from the origin. On any fundamental period defined by the lattice, the boundary values and normal derivatives of G^a tend to the quasi-periodic boundary conditions as $a \to \infty$. On the other hand, the sum obtained by replacing the truncation in (24) with the spatially dependent one $\chi(\frac{x+d_1 m}{a}, \frac{y+d_2 n}{a})$ is quasi-periodic but does not satisfy the Helmholtz equation. It is the partial Floquet transform of the function $\chi(x,y)e^{ikr}/r$, namely, an infinite sum of monopole-source Helmholtz fields situated on the lattice, each truncated gently, far from its source, by a smooth truncation. As $a \to \infty$, each contribution approaches a true radiating Helmholtz field.

The following theorem establishes the super-algebraic convergence of the smoothly truncated lattice sum to the periodic Green function. The convergence is demonstrated numerically in Figures 1 and 2, in which the slope on a log-log graph of the error against the truncation radius increases. One also observes that the convergence is slow near Wood frequencies.

Theorem 3.1 (Green function at non-Wood frequencies; super-algebraic convergence)**.** *Let $\chi(s,t)$ be a smooth truncation function equal to 1 for $s^2+t^2 < A^2 > 0$ and equal to 0 for $s^2+t^2 > B^2$. If $\gamma_{j\ell} \neq 0$ for all $(j,\ell) \in \mathbb{Z}^2$, then the functions*

$$G_k^a(x,y,z) = \frac{1}{4\pi} \sum_{m,n\in\mathbb{Z}} \frac{e^{ik\left((x+md_1)^2+(y+nd_2)^2+z^2\right)^{1/2}}}{\left((x+md_1)^2+(y+nd_2)^2+z^2\right)^{1/2}} e^{-i(\alpha m d_1 + \beta n d_2)} \chi\left(\tfrac{md_1}{a}, \tfrac{nd_2}{a}\right)$$

converge to the radiating quasi-periodic Green function $G_k^{qper}(x,y,z)$ super-algebraically as $a \to \infty$. Specifically, for each compact set $K \in \mathbb{R}^3$, there exist constants $C_n = C_n(k)$ such that

$$|G_k^a(x,y,z) - G_k^{qper}(x,y,z)| < \frac{C_n(k)}{a^n}$$

if a is sufficiently large and $(x,y,z) \in K$, $(x,y,z) \notin d_1\mathbb{Z} \times d_2\mathbb{Z} \times \{0\}$.

Proof. The proof proceeds by first using the Poisson Summation Formula to prove that $G_k^a(\mathbf{x})$ is a Cauchy family as $a \to \infty$ with super-algebraic convergence on compact subsets of $\mathbb{R}^3$. One then shows that the limit is independent of the truncation function and uses this fact to prove the quasi-periodicity of the limit. That $G_k^{qper}(\mathbf{x})$ is a fundamental solution follows from the definition of $G_k^a(\mathbf{x})$ as a finite superposition of radial Green functions. That $G_k^{qper}(\mathbf{x})$ is radiating is a consequence of the principle of vanishing absorption. The proof is broken into four steps.

Step 1. First we prove that there are constants C_n such that, if a is sufficiently large and $b > a$, then for $\mathbf{x} \in K$,

$$\left|G_k^b(\mathbf{x}) - G_k^a(\mathbf{x})\right| < \frac{C_n(k)}{a^n},$$

and thus, as $a \to \infty$, $G_k^a(\mathbf{x})$ converges to a function $G(\mathbf{x})$ with $\left|G(\mathbf{x}) - G_k^a(\mathbf{x})\right| \leq \frac{C_n(k)}{a^n}$ for all $\mathbf{x} \in K$ (with $\mathbf{x} \notin d_1\mathbb{Z} \times d_2\mathbb{Z} \times \{0\}$).

The difference

$$
\begin{aligned}
&G_k^b(\mathbf{x}) - G_k^a(\mathbf{x}) = \\
&\quad = \frac{1}{4\pi} \sum_{m,n\in\mathbb{Z}} \frac{e^{ik\left((x+md_1)^2+(y+nd_2)^2+z^2\right)^{1/2}}}{\left((x+md_1)^2+(y+nd_2)^2+z^2\right)^{1/2}} e^{-i(\alpha m d_1 + \beta n d_2)} \left(\chi(\tfrac{md_1}{b}, \tfrac{nd_2}{b}) - \chi(\tfrac{md_1}{a}, \tfrac{nd_2}{a})\right),
\end{aligned}
$$

for fixed $\mathbf{x}$ is a lattice sum of a function of m and n that is supported in $aA < \sqrt{(md_1)^2 + (nd_2)^2} < bB$. It is smooth in m and n when these variables take on general real values. Application of the Poisson Summation Formula, with $md_1 = \hat{x}$ and $nd_2 = \hat{y}$, yields

$$
\begin{aligned}
&G_k^b(\mathbf{x}) - G_k^a(\mathbf{x}) = \\
&\frac{1}{4\pi}\frac{1}{d_1 d_2} \sum_{j,\ell\in\mathbb{Z}} \iint_{\mathbb{R}^2} \frac{e^{ik\left((x+\hat{x})^2+(y+\hat{y})^2+z^2\right)^{1/2}}}{\left((x+\hat{x})^2+(y+\hat{y})^2+z^2\right)^{1/2}} e^{-i\left((\alpha+\frac{2\pi}{d_1}j)\hat{x}+(\beta+\frac{2\pi}{d_2}\ell)\hat{y}\right)} \left(\chi(\tfrac{\hat{x}}{b}, \tfrac{\hat{y}}{b}) - \chi(\tfrac{\hat{x}}{a}, \tfrac{\hat{y}}{a})\right) d\hat{x}d\hat{y}.
\end{aligned}
$$

By the change of variables $s = (\hat{x}+x)/a$ and $t = (\hat{y}+y)/a$, this becomes

$$
\begin{aligned}
G_k^b(\mathbf{x}) - G_k^a(\mathbf{x}) &= \frac{1}{4\pi}\frac{a}{d_1 d_2} \sum_{j,\ell\in\mathbb{Z}} e^{i\left((\alpha+\frac{2\pi}{d_1}j)x+(\beta+\frac{2\pi}{d_2}\ell)y\right)} \times \\
&\iint_{\mathbb{R}^2} \frac{\chi(\frac{as-x}{b}, \frac{at-y}{b}) - \chi(s-\frac{x}{a}, t-\frac{y}{a})}{\sqrt{s^2+t^2+\left(\frac{z}{a}\right)^2}} \, e^{iak\sqrt{s^2+t^2+\left(\frac{z}{a}\right)^2}} \, e^{-ia\left((\alpha+\frac{2\pi}{d_1}j)s+(\beta+\frac{2\pi}{d_2}\ell)t\right)} ds\, dt\,.
\end{aligned}
$$

The double integral can be written as

$$
I_{j\ell} \;=\; \iint_{\mathbb{R}^2} \frac{\phi_{a,b}(s,t)}{\sqrt{s^2+t^2}} \, e^{iak\sqrt{s^2+t^2}} \, e^{-ia\left((\alpha+\frac{2\pi}{d_1}j)s+(\beta+\frac{2\pi}{d_2}\ell)t\right)} ds\, dt,
$$

in which

$$
\phi_{a,b}(s,t) \;=\; \frac{\chi(\frac{as-x}{b}, \frac{at-y}{b}) - \chi(s-\frac{x}{a}, t-\frac{y}{a})}{\sqrt{1+(\frac{z}{a\sqrt{s^2+t^2}})^2}} \, \exp\left(\frac{ik}{a\sqrt{s^2+t^2}} \frac{z^2}{1+\sqrt{1+(\frac{z}{a\sqrt{s^2+t^2}})^2}} \right). \tag{25}
$$

Setting $\langle \alpha + \frac{2\pi}{d_1}j, \beta + \frac{2\pi}{d_2}\ell \rangle = \xi \langle \cos\gamma, \sin\gamma \rangle$ with $\xi \geq 0$, the integral can be written as

$$
I_{j\ell} = \iint_{\mathbb{R}^2} f(s,t) e^{ia\xi g(s,t)} ds\, dt,
$$

in which

$$
\begin{aligned}
f(s,t) \;&=\; \frac{\phi_{a,b}(s,t)}{\sqrt{s^2+t^2}}\,, \\
g(s,t) \;&=\; \frac{k}{\xi}\sqrt{s^2+t^2} - (s\cos\gamma + t\sin\gamma)\,.
\end{aligned}
$$

The gradient of g

$$\nabla g(s,t) = \frac{k}{\xi}\left\langle \frac{s}{\sqrt{s^2+t^2}}\,,\ \frac{t}{\sqrt{s^2+t^2}} \right\rangle - \langle \cos\gamma,\ \sin\gamma\rangle$$

is bounded below and above as long as $k \neq \xi$ (recall ξ and k are both non-negative), which is guaranteed by the assumption that $\gamma_{j\ell} \neq 0$ for all $(j,\ell) \in \mathbb{Z}^2$,

$$\left|1 - \frac{k}{\xi}\right| \leq \|\nabla g\| \leq 1 + \frac{k}{\xi}\,. \tag{26}$$

Define the operator

$$L := \frac{\nabla g \cdot \nabla}{ia\xi\|\nabla g\|^2}\,,$$

and observe that it fixes $e^{ia\xi g(s,t)}$. Since $f(s,t)$ is smooth and has compact support, one obtains by repeated integration by parts

$$\begin{aligned} I_{j\ell} &= \iint\limits_{\mathbb{R}^2} f(s,t)e^{ia\xi g(s,t)}ds\,dt = \iint\limits_{\mathbb{R}^2} f(s,t)Le^{ia\xi g(s,t)}ds\,dt = \\ &= \frac{i}{a\xi}\iint\limits_{\mathbb{R}^2} \nabla\cdot\frac{f\,\nabla g}{\|\nabla g\|^2}e^{ia\xi g(s,t)}ds\,dt = \left(\frac{i}{a\xi}\right)^n \iint\limits_{\mathbb{R}^2} f_n(s,t)e^{ia\xi g(s,t)}ds\,dt, \end{aligned} \tag{27}$$

in which

$$f_0 = f, \tag{28}$$

$$f_{n+1} = \nabla\cdot\frac{f_n\,\nabla g}{\|\nabla g\|^2}, \quad n \geq 0. \tag{29}$$

In polar coordinates $(s,t) = r(\cos\theta,\sin\theta)$, the gradient of g and its square magnitude are

$$\begin{aligned} \nabla g &= \left\langle \frac{k}{\xi}\cos\theta - \cos\gamma,\ \frac{k}{\xi}\sin\theta - \sin\gamma \right\rangle, \\ \|\nabla g\|^2 &= \frac{k^2}{\xi^2} + 1 - 2\frac{k}{\xi}\cos(\theta-\gamma). \end{aligned}$$

To prove that

$$f_n(s,t) = \mathcal{O}\left(r^{-n-1}\right), \quad r\to\infty,$$

one establishes that, for $r > B$, f_n has the form

$$f_n(s,t) = \frac{P_n(\cos\theta,\sin\theta)}{\|\nabla g(s,t)\|^{4(2^n-1)}}h_n(r), \quad r > B.$$

in which P_n is a polynomial in two variables and h_n has the desired decay,

$$h_n(r) = \frac{1}{r^{n+1}}\tilde{h}_n(r), \quad \tilde{h}_n \text{ analytic at } r=\infty.$$

For $n=0$, this follows from (25) and $f_0 = \phi_{a,b}/r$. Induction on n is made possible by the observation that $\|\nabla g\|^2$ and the components of ∇g are polynomials in $\cos\theta$ and $\sin\theta$ and that the gradient of such a polynomial decays as $1/r$:

$$\nabla P(\cos\theta,\sin\theta) = \frac{1}{r}\left\langle Q_1(\cos\theta,\sin\theta),\ Q_2(\cos\theta,\sin\theta)\right\rangle,$$

in which Q_1 and Q_2 are polynomials.

Finally, the sum we are seeking is

$$G^b_k(\mathbf{x}) - G^a_k(\mathbf{x}) \;=\; \frac{i^n}{4\pi a^{n-1}}\frac{1}{d_1 d_2}\sum_{j,\ell\in\mathbb{Z}} e^{i\left((\alpha+\frac{2\pi}{d_1}j)x+(\beta+\frac{2\pi}{d_2}\ell)y\right)}\times$$
$$\frac{1}{((\alpha+\frac{2\pi}{d_1}j)^2+(\beta+\frac{2\pi}{d_2}\ell)^2\,)^{n/2}}\iint_{\mathbb{R}^2} f_n(s,t)e^{ia\sqrt{(\alpha+\frac{2\pi}{d_1}j)^2+(\beta+\frac{2\pi}{d_2}\ell)^2}\,g(s,t)}ds\,dt.$$

The integrals are absolutely convergent for $n\geq 2$ and bounded by a constant C_n that depends only on the compact set K and the wavenumber k, that is $C_n = C_n(k)$; in particular, it does not depend on b. The sum converges for $n\geq 3$.

Step 2. Next, we prove that the limit $G(\mathbf{x})$ is independent of the truncation function $\chi(s,t)$, and if χ_1 and χ_2 are two truncation functions giving rise to two families of functions $G^a_1(\mathbf{x})$ and $G^a_2(\mathbf{x})$, then for each compact set $K\subset\mathbb{R}^3$, there are constants C_n such that

$$\sup_{\mathbf{x}\in K}|G^a_1(\mathbf{x})-G^a_2(\mathbf{x})| \;<\; \frac{C_n(k)}{a^n}\sup_{s,t\in\mathbb{R}}|\chi_1^{(n)}(s,t)-\chi_2^{(n)}(s,t)|\,.$$

The proof proceeds as in Step 1, but with $\chi(\frac{md_1}{b},\frac{nd_2}{b})-\chi(\frac{md_1}{a},\frac{nd_2}{a})$ replaced by $\chi_1(\frac{md_1}{a},\frac{nd_2}{a})-\chi_2(\frac{md_1}{a},\frac{nd_2}{a})$, and hence $\phi_{a,b}$ replaced by

$$\phi_a(s,t) \;=\; \frac{\chi_1(s-\frac{x}{a},t-\frac{y}{a})-\chi_2(s-\frac{x}{a},t-\frac{y}{a})}{\sqrt{1+(\frac{z}{a\sqrt{s^2+t^2}})^2}}\,\exp\left(\frac{ik}{a\sqrt{s^2+t^2}}\,\frac{z^2}{1+\sqrt{1+(\frac{z}{a\sqrt{s^2+t^2}})^2}}\right) \tag{30}$$

and $f(s,t)$ by

$$f(s,t) \;=\; \frac{\phi_a(s,t)}{\sqrt{s^2+t^2}}\,,$$

and f_n defined by the same recursion as above, to obtain

$$G^a_1(\mathbf{x}) - G^a_2(\mathbf{x}) \;=\; \frac{i^n}{4\pi a^{n-1}}\sum_{j,\ell\in\mathbb{Z}} e^{i\left((\alpha+\frac{2\pi}{d_1}j)x+(\beta+\frac{2\pi}{d_2}\ell)y\right)}\times$$
$$\frac{1}{((\alpha+\frac{2\pi}{d_1}j)^2+(\beta+\frac{2\pi}{d_2}\ell)^2\,)^{n/2}}\iint_{\mathbb{R}^2} f_n(s,t)e^{ia\sqrt{(\alpha+\frac{2\pi}{d_1}j)^2+(\beta+\frac{2\pi}{d_2}\ell)^2}\,g(s,t)}ds\,dt.$$

Step 3. Now, we prove that the function $G(\mathbf{x})$ is a Green function of the Helmholtz equation, and it is quasi-periodic with periodicity lattice $\mathbb{Z}^2\times\{0\}\subset\mathbb{R}^3$ and Bloch vector (κ_1,κ_2).

First, if a is sufficiently large, then, for each lattice point (md_1,nd_2) in K, $\chi(\frac{md_1}{a},\frac{nd_2}{a})=1$, and thus the (m,n) term

$$h_{mn}(\mathbf{x}) \;=\; \frac{e^{ikr_{mn}}}{r_{mn}}e^{i(\alpha md_1+\beta nd_2)}, \qquad r_{mn} \;=\; \left((md_1+x)^2+(nd_2+y)^2+z^2\right)^{1/2},$$

in the lattice sum for $G^a(\mathbf{x})$ satisfies

$$\nabla^2 h_{mn}(\mathbf{x})+k^2h_{mn}(\mathbf{x}) \;=\; -\delta(\mathbf{x}+(md_1,nd_2,0))\,e^{i(\alpha md_1+\beta nd_2)}$$

for all $\mathbf{x} \in \mathbb{R}^3$. For the finitely many pairs $(md_1, nd_2) \notin K$ such that $\chi(\frac{md_1}{a}, \frac{nd_2}{a}) \neq 0$, the (m,n) term in the lattice sum for $G^a(\mathbf{x})$ satifies

$$\nabla^2 G(\mathbf{x}) + k^2 G(\mathbf{x}) = 0$$

for all $\mathbf{x} \in K$. Thus for $\mathbf{x} \in K$ and a sufficiently large, one has

$$\nabla^2 G(\mathbf{x}) + k^2 G(\mathbf{x}) \;=\; - \sum_{m,n\in\mathbb{Z}} \delta(\mathbf{x} - (md_1, nd_2, 0))\, e^{i(\alpha m d_1 + \beta n d_2)}\,.$$

To prove that $G(\mathbf{x})$ is quasi-periodic, let $\mathbf{x}$ and $\mathbf{x} + (m'd_1, n'd_2, 0)$ be in K and observe that

$$G_k^a(\mathbf{x}) = \frac{1}{4\pi} \sum_{m,n\in\mathbb{Z}} \frac{ikr_{mn}}{r_{mn}} e^{i(\alpha m d_1 + \beta n d_2)} \chi(\tfrac{md_1}{a}, \tfrac{nd_2}{a})$$

and

$$\begin{aligned} G_k^a(\mathbf{x} + (m'd_1, n'd_2, 0)) &= \frac{1}{4\pi} \sum_{m,n\in\mathbb{Z}} \frac{e^{ikr_{m+m',n+n'}}}{r_{m+m',n+n'}} e^{-i(\alpha m d_1 + \beta n d_2)} \chi(\tfrac{md_1}{a}, \tfrac{nd_2}{a}) \\ &= e^{i(\alpha m d_1' + \beta n d_2')} \frac{1}{4\pi} \sum_{m,n\in\mathbb{Z}} \frac{e^{ikr_{mn}}}{r_{mn}} e^{-i(\alpha m d_1 + \beta n d_2)} \chi(\tfrac{(m-m')d_1}{a}, \tfrac{(n-n')d_2}{a})\,. \end{aligned}$$

The latter expression differs from that for $G_k^a(\mathbf{x})$ only in the prefactor and in the modified truncation function $\chi(s - \frac{m'}{a}, t - \frac{n'}{a})$ which tends to $\chi(s,t)$ uniformly in all its derivatives as $a \to \infty$. By Step 2, we conclude that $G_k^a(\mathbf{x}+(m'd_1, n'd_2, 0)) - e^{i(\alpha m' d_1 + \beta n' d_2)} G_k^a(\mathbf{x})$ tends to zero as $a \to \infty$, which means that $G(\mathbf{x} + (m'd_1, n'd_2, 0)) = e^{i(\alpha m' d_1 + \beta n' d_2)} G(\mathbf{x})$.

Step 4. That $G(\mathbf{x})$ is radiating is proved by means of the principle of vanishing absorption. Perturbing k by a small positive imaginary part effects exponential decay in the radial Green function, which, in turn, results in a quasi-periodic Green function $G(\mathbf{x})$ that exhibits exponential decay as $|z| \to \infty$. The continuity of $G(\mathbf{x})$ in the uniform norm on compact sets of $\mathbb{R}^3$ as a function k guarantees that $G(\mathbf{x})$ is the unique radiating quasi-periodic Green function G_k^{qper} for real $k > 0$. ■

4 Lattice sums at Wood frequencies

To deal with the divergence of the lattice sum for the quasi-periodic Green function at Wood frequencies, we employ a combination of shifts of $G_k^{qper}(\mathbf{x})$ in the z variable. This introduces poles at several perpendicular shifts of the integer lattice $\mathbb{Z}^2$,

$$G_k^{qper,p}(\mathbf{x}) = \sum_{q=0}^{p} a_{pq} G_k^{qper}\left(\mathbf{x} + (0,0,qd)\right)\,.$$

This sum makes sense at non-Wood parameters (k, α, β) when $\gamma_{j\ell} \neq 0$ for all (j, ℓ) and thus G_k^{qper} exists. In fact, if the sum over q and the lattice sum for G_k^{qper} are interchanged, it will converge even *at* Wood parameters, provided the weights a_{pq} are chosen appropriately,

$$G_k^{qper,p}(\mathbf{x}) = \frac{1}{4\pi} \sum_{m,n\in\mathbb{Z}} e^{-i(\alpha m d_1 + \beta n d_2)} \sum_{q=0}^{p} a^{pq} \frac{e^{ikr_{mn}^{pq}}}{r_{mn}^{pq}}\,, \tag{31}$$

in which the r_{mn}^{pq} are defined by

$$r_{mn}^{pq} = \sqrt{(x+md_1)^2 + (y+nd_2)^2 + (z+qd)^2}\,.$$

We then truncate the sum by a smooth function $\chi(x/a, y/a)$. Theorem 4.3 asserts that the sum converges algebraically as $C/a^{\lceil p/2\rceil - 1/2}$.

As a function of $\mathbf{x}$ for fixed $\mathbf{x}'$, $G_k^{qper,p}(\mathbf{x}-\mathbf{x}')$ has $p+1$ poles with z-values at

$$z'^{pq} \;=\; z' - qd, \qquad q = 0, \dots p\,,$$

which are below the domain of interest for a problem of reflection by a periodic grating.

The weights a_{pq} are chosen to be the alternating binomial coefficients

$$a_{pq} = (-1)^q \binom{p}{q}, \qquad 0 \le q \le p\,,$$

because they realize a p^{th} difference, that is, if the p^{th} derivative of a function f is continuous, then

$$\begin{aligned}\sum_{q=0}^{p} a_{pq} f(\epsilon(a+qd)) \;&=\; \sum_{k=0}^{p-1} \epsilon^k d^k f^{(k)}(a) \sum_{q=0}^{p} a_{pq} q^k + \epsilon^p d^p \sum_{q=0}^{p} a_{pq} q^p f^{(p)}(x_q) \\ &=\; \epsilon^p d^p \sum_{q=0}^{p} a_{pq} q^p f^{(p)}(x_q)\,, \qquad x_q \in [\epsilon a, \epsilon(a+qd)] \subset [0, \epsilon(a+pd)]. \qquad (32)\end{aligned}$$

Before proving the algebraic convergence of (31), which takes place to high order for adequately large p, we prove that it is well defined and that the boundary-integral equation discussed in section 2 is well posed when $G_k^{qper,p}(\mathbf{x})$, after a simple modification, is used in place of G_k (Theorem 4.1).

4.1 Fourier form of the modified Green function

We will show that $G_k^{qper,p}(\mathbf{x})$ is well defined and satisfies the Helmholtz equation away from its singularities at r_{mn}^{pq}; more precisely,

$$\nabla^2 G_k^{qper,p} + k^2 G_k^{qper,p} \;=\; -\sum_{m,n\in\mathbb{Z}} \sum_{q=0}^{p} e^{i(\alpha m d_1 + \beta n d_2)} \delta(\mathbf{x} - \mathbf{x}'_{mnq})\,.$$

In fact, we will show this for a regular modification of $G_k^{qper,p}$, obtained by adding a solution of the homogeneous Helmholtz equation. To this end, it is necessary to work with the Fourier form of the Green functions.

If $\gamma_{jl} \neq 0$ for all (j,ℓ), the doubly-periodic radiating Green function has the Fourier series

$$G_k^{qper}(\mathbf{x}) = \frac{i}{2d_1 d_2} \sum_{j,\ell\in\mathbb{Z}} e^{i(\alpha_j x + \beta_\ell y)} \frac{1}{\gamma_{j\ell}} e^{i\gamma_{j\ell}|z|}\,.$$

Suppose that $\gamma_{j\ell}$ tends to 0 for some (j,ℓ) (as k, α, and β tend to suitable values). The z-dependent factor of the $j\ell$-term can be split into analytic and nonanalytic parts:

$$\frac{1}{\gamma_{j\ell}} e^{i\gamma_{j\ell}|z|} = \frac{1}{\gamma_{j\ell}} \cos(\gamma_{j\ell}\, z) + \frac{i}{\gamma_{j\ell}} \sin(\gamma_{j\ell}|z|)\,. \qquad (33)$$

The first term diverges as $\gamma_{j\ell} \to 0$, while the second term tends to $i|z|$. By using a suitable linear combination of shifts of this function, the first term can be made to vanish.

Applying the p^{th} difference (32) to the function (33) yields an expression that is continuous in (k, α, β) in a punctured neighborhood of a triple (k_0, α_0, β_0) at which $\gamma_{j\ell} = 0$, and the analytic part vanishes at (k_0, α_0, β_0):

$$\sum_{q=0}^{p} \frac{a_{pq}}{\gamma_{j\ell}} e^{i\gamma_{j\ell}|z+qd|} = \frac{1}{\gamma_{j\ell}} \sum_{q=0}^{p} a_{pq} \cos(\gamma_{j\ell}(z+qd)) + i \sum_{q=0}^{p} \frac{a_{pq}}{\gamma_{j\ell}} \sin(\gamma_{j\ell}|z+qd|)$$
$$\longrightarrow\ 0 + i \sum_{q=0}^{p} a_{pq}|z+qd| \qquad (\gamma_{j\ell} \to 0,\ p \geq 1). \quad (34)$$

Thus the following function is well defined, even when $\gamma_{j\ell} = 0$ for some pairs (j, ℓ) when the Green function $G_k^{qper}(\mathbf{x})$ does not exist:

$$G_k^{qper,p}(\mathbf{x}) = \frac{i}{2d_1d_2} \sum_{j\ell} e^{i(\alpha_j x + \beta_\ell y)} \frac{1}{\gamma_{j\ell}} \sum_{q=0}^{p} a_{pq} e^{i\gamma_{j\ell}|z+qd|}\,.$$

If $\gamma_{j\ell} \neq 0$ for each pair (j, ℓ), then $G_k^{qper,p}$ is a combination of "copies" of the radiating periodic Green function with poles shifted perpendicular to the integer lattice $\mathbb{Z}^2$:

$$G_k^{qper,p}(\mathbf{x}) = \sum_{q=0}^{p} a_{pq} G_k^{qper}(\mathbf{x} + (0,0,qd)).$$

For z such that $z + qd > 0$ for all $0 \leq q \leq p$, the right-hand side of equation (34) vanishes, since $\sum_{q=0}^{p} a_{pq} = 0$ and $\sum_{q=0}^{p} q a_{pq} = 0$. Thus, if $\gamma_{j\ell} = 0$, the (j, ℓ) Fourier component is not represented in the far field. To deal with this, we follow [3] and introduce a modification $\tilde{G}_k^{per,p}$ of $G_k^{per,p}$ that is outgoing for $z \to \infty$, including at Wood frequencies:

$$\tilde{G}_k^{qper,p}(\mathbf{x}) \;=\; G_k^{qper,p}(\mathbf{x}) \;+\; v(\mathbf{x}),$$

where we have added a regular Helmholtz field $v(\mathbf{x}, \mathbf{x}')$,

$$v(\mathbf{x}) = \frac{i}{2d_1d_2} \sum_{j,\ell \in \mathbb{Z}} b_{j\ell}\, e^{i(\alpha_j x + \beta_\ell y)} e^{i\gamma_{j\ell}\, z}\,, \qquad (b_{j\ell} = 0 \text{ for all } j, \ell \text{ sufficiently large})$$

with coefficients $b_{j\ell}$ nonvanishing for those (j, ℓ) such that $\gamma_{j\ell}$ is small. In particular, $b_{j\ell} \neq 0$ for all (j, ℓ) such that $\gamma_{j\ell} = 0$; denote this subset of $\mathbb{Z}^2$ by U. We also demand that $b_{j\ell} = 0$ for all but a finite number of pairs (j, ℓ). If all $\gamma_{j\ell}$ are nonzero, then

$$\tilde{G}_k^{qper,p}(\mathbf{x}) \;=\; \sum_{q=0}^{p} a_{pq} G_k^{qper}(\mathbf{x} + (0,0,qd)) + v(\mathbf{x})\,.$$

The function $\tilde{G}_k^{qper,p}(\mathbf{x})$ is (α, β) quasi-periodic with quasi-periods d_1 and d_2 in x and y and has poles on $p+1$ shifts of the two-dimensional lattice $\mathbb{Z}^2$:

$$\nabla^2 \tilde{G}_k^{qper,p} + k^2 \tilde{G}_k^{qper,p} \;=\; -\sum_{m,n \in \mathbb{Z}} \sum_{q=0}^{p} e^{i(\alpha m d_1 + \beta n d_2)} \delta(\mathbf{x} - \mathbf{x}'_{mnq})\,,$$

in which

$$\mathbf{x}'_{mnq} = \mathbf{x}' - (md_1, nd_2, qd)\,.$$

4.2 Integral equation formulations at and near Wood frequencies

As before, let Γ denote one period of a $2D$-periodic surface (a grating) Γ_{per} in $\mathbb{R}^3$ with periods d_1 and d_2 in x and y defined by means of a periodic C^1 function $f:\mathbb{R}^2\to\mathbb{R}$ by $z=f(x,y)$, with

$$z_- < f(x,y) < z_+\,,$$

and let the normal vector n to Γ be directed into the upper part Γ_+ of $\mathbb{R}^2$ where $z>f(x,y)$.

Using the Green function $\tilde{G}_k^{qper,p}$ we have just introduced, we look for a scattered field in the form of a combined single- and double-layer potential,

$$u(\mathbf{x}) := \int_{\Gamma_{per}} \phi(\mathbf{x}')\left[i\eta\,\tilde{G}_k^{qper,p}(\mathbf{x}-\mathbf{x}') + \xi\,\frac{\partial \tilde{G}_k^{qper,p}(\mathbf{x}-\mathbf{x}')}{\partial \mathbf{n}(\mathbf{x}')}\right] ds(\mathbf{x}') \tag{35}$$

of an unknown periodic density ϕ defined on Γ_{per}. By classical potential theory, this function is quasi-periodic and outgoing, and it satisfies the Helmholtz equation in $\mathbb{R}^3\setminus\bigcup_{q=0}^p(\Gamma_{\rm per}-(0,0,qd))$, that is, it is regular off the $p+1$ shifted copies of $\Gamma_{\rm per}$. One can derive easily a periodic formulation of the scattering problem by extracting an appropriate phase from $\tilde{G}_k^{qper,p}$ in order to render it periodic.

Theorem 4.1. *If $u(\mathbf{x})=0$ in (35) for all $\mathbf{x}\in\Gamma$, then $\phi(\mathbf{x})=0$ for all $\mathbf{x}\in\Gamma$, provided that $\eta/\xi<0$ and that $d\notin D$ (in the definition of $\tilde{G}_k^{qper,p}$, with $p\geq 1$), where D is a subset of $\mathbb{R}$ such that $D\cap[0,d_0]$ is finite for each d_0.*

Proof. Let U be the set of all pairs $(j,\ell)\in\mathbb{Z}^2$ for which $\gamma_{j\ell}=0$. Then $\tilde{G}_k^{qper,p}(\mathbf{x}-\mathbf{x}')$ has the representation

$$\begin{aligned}\tilde{G}_k^{qper,p}(\mathbf{x}) = \frac{i}{2d_1d_2}\sum_{(j,\ell)\notin U} e^{i(\alpha_j x+\beta_\ell y)}\frac{1}{\gamma_{j\ell}}\sum_{q=0}^{p} a_{pq}e^{i\gamma_{j\ell}|z+qd|} \;+\; v_1(\mathbf{x}) + \\ + \frac{i}{2d_1d_2}\sum_{(j,\ell)\in U} e^{i(\alpha_j x+\beta_\ell y)}i\sum_{q=0}^{p} a_{pq}|z+qd| \;+\; v_2(\mathbf{x})\,,\end{aligned}$$

in which $v=v_1+v_2$ and v_2 simplifies to a function that is independent of z:

$$\begin{aligned} v_1(\mathbf{x}) &= \frac{i}{2d_1d_2}\sum_{(j,\ell)\notin U} b_{j\ell}\,e^{i(\alpha_j x+\beta_\ell y)}e^{i\gamma_{j\ell}\,z}\,,\\ v_2(\mathbf{x}) &= \frac{i}{2d_1d_2}\sum_{(j,\ell)\in U} b_{j\ell}\,e^{i(\alpha_j x+\beta_\ell y)}\,.\end{aligned}$$

Observe that $G_k^{qper,p}(\mathbf{x})$ can be written as a sum of shifted Green functions that do not satisfy the outgoing condition because of the linearly growing harmonics $(j,\ell)\in I_2$. But $\tilde{G}_k^{qper,p}-v$ itself *does* satisfy the outgoing condition because these linear harmonics mutually cancel for large enough $|z|$ ($z>0$ and $z<-pd$). One has

$$\tilde{G}_k^{qper,p}(\mathbf{x}) \;=\; \sum_{q=0}^{p} a_{pq}B(\mathbf{x}+(0,0,qd)) + v(\mathbf{x}),$$

in which

$$B(\mathbf{x}) \;=\; \frac{i}{2d_1d_2}\sum_{(j,\ell)\notin U} e^{i(\alpha_j x+\beta_\ell y)}\,\frac{1}{\gamma_{j\ell}}e^{i\gamma_{j\ell}|z|} \;+\; \frac{i}{2d_1d_2}\sum_{(j,\ell)\in U} e^{i(\alpha_j x+\beta_\ell y)} i|z|$$

is a quasi-periodic function Green function, which is not outgoing because of the terms containing $|z|$ as a factor.

Now set

$$\begin{aligned}
u^0(\mathbf{x}) \;&=\; \int_\Gamma \phi(\mathbf{x}')\left[i\eta\, B(\mathbf{x}-\mathbf{x}') + \xi\,\frac{\partial B(\mathbf{x}-\mathbf{x}')}{\partial\mathbf{n}(\mathbf{x}')}\right] ds(\mathbf{x}')\,,\\
v^0(\mathbf{x}) \;&=\; \int_\Gamma \phi(\mathbf{x}')\left[i\eta\, v(\mathbf{x}-\mathbf{x}') + \xi\,\frac{\partial\, v(\mathbf{x}-\mathbf{x}')}{\partial\mathbf{n}(\mathbf{x}')}\right] ds(\mathbf{x}')\,,
\end{aligned}$$

so that

$$u(\mathbf{x}) \;=\; \sum_{q=0}^{p} a_{pq} u^0(\mathbf{x}+(0,0,qd)) + v^0(\mathbf{x})\,. \tag{36}$$

In its Fourier expansion for $z>z_+$, u^0 has the form

$$u^0(\mathbf{x}) = \sum_{j,\ell\in\mathbb{Z}} u^{0+}_{j\ell}(z)\, e^{i(\alpha_j x+\beta_\ell y)} \qquad (z>z_+)\,,$$

in which the z-dependent coefficients are given by

$$\begin{aligned}
u^{0+}_{j\ell}(z) \;&=\; c_{j\ell}\frac{1}{\gamma_{j\ell}}e^{i\gamma_{j\ell}z} \qquad \text{for } (j,\ell)\notin U\,,\\
u^{0+}_{j\ell}(z) \;&=\; i\big(c_{j\ell}z - c'_{j\ell}\big) + c''_{j\ell} \qquad \text{for } (j,\ell)\in U\,,
\end{aligned}$$

with

$$\begin{aligned}
c_{j\ell} \;&=\; \frac{1}{2d_1d_2}\left[-\eta\int_\Gamma \phi(\mathbf{x}')e^{-i(\alpha_j x'+\beta_\ell y')}e^{-i\gamma_{j\ell}z'}ds(\mathbf{x}') + \right.\\
&\qquad \left. +\,\xi\int_\Gamma \phi(\mathbf{x}')(\alpha_j,\beta_\ell,\gamma_{j\ell})\cdot\mathbf{n}(\mathbf{x}')e^{-i(\alpha_j x'+\beta_\ell y')}e^{-i\gamma_{j\ell}z'}ds(\mathbf{x}')\right]\,,\\
c'_{j\ell} \;&=\; \frac{1}{2d_1d_2}\left[-\eta\int_\Gamma \phi(\mathbf{x}')\, z'\, e^{-i(\alpha_j x'+\beta_\ell y')}ds(\mathbf{x}') + \right.\\
&\qquad \left. +\,\xi\int_\Gamma \phi(\mathbf{x}')(\alpha_j,\beta_\ell,0)\cdot\mathbf{n}(\mathbf{x}')\, z'\, e^{-i(\alpha_j x'+\beta_\ell y')}ds(\mathbf{x}')\right]\,,\\
c''_{j\ell} \;&=\; \frac{\xi}{2d_1d_2}\int_\Gamma \phi(\mathbf{x}')(0,0,1)\cdot\mathbf{n}(\mathbf{x}')\, e^{-i(\alpha_j x'+\beta_\ell y')}ds(\mathbf{x}')\,.
\end{aligned}$$

The expansion of v^0 is simple:

$$v^0(\mathbf{x}) \;=\; \sum_{(j,\ell)\in U} b_{j\ell}\, c_{j\ell}\, e^{i(\alpha_j x+\beta_\ell y)}e^{i\gamma_{j\ell}z} \quad (z>z_+)\,.$$

The field $u(\mathbf{x})$ (see (36)) has a Fourier expansion

$$u(\mathbf{x}) \;=\; \sum_{j\ell} e^{i(\alpha_j x+\beta_\ell y)} u_{j\ell}(z)\,,$$

with z-dependent coefficients given for $z > z_+$ by

$$u_{j\ell}(z) \;=\; c_{j\ell}\left(\frac{1}{\gamma_{j\ell}}\sum_{q=0}^{p} a_{pq}e^{i\gamma_{j\ell}qd} + b_{j\ell}\right)e^{i\gamma_{j\ell}z}, \qquad [(j,\ell)\notin U,\; z>z_+]$$

$$u_{j\ell}(z) \;=\; \sum_{q=0}^{p} a_{pq}\left(i\left(c_{j\ell}(z+qd) - c'_{j\ell}\right) + c''_{j\ell}\right) + b_{j\ell}\,c_{j\ell}. \qquad [(j,\ell)\in U,\; z>z_+]$$

Since the a_{pq} are defined as the alternating binomial coefficients, one has

$$\sum_{q=0}^{p} a_{pq}e^{i\gamma_{j\ell}qd} \;=\; \left(1-e^{i\gamma_{j\ell}d}\right)^p\,,$$

$$\sum_{q=0}^{p} a_{pq} = 0\,,$$

$$\sum_{q=0}^{p} q a_{pq} = \begin{cases} -1\,, & p=1\,,\\ 0\,, & p\geq 2\,,\end{cases}$$

which simplifies the coefficients to

$$u_{j\ell}(z) \;=\; c_{j\ell}\left(\frac{1}{\gamma_{j\ell}}\left(1-e^{i\gamma_{j\ell}d}\right)^p + b_{j\ell}\right)e^{i\gamma_{j\ell}z}, \qquad [(j,\ell)\notin U,\; z>z_+]$$

$$u_{j\ell}(z) \;=\; c_{j\ell}(-id\,\delta_{p1} \,+\, b_{j\ell})\,, \qquad [(j,\ell)\in U,\; z>z_+]$$

in which δ_{p1} is 1 for $p=1$ and 0 for $p\geq 2$.

Assume now that $u(\mathbf{x}) = 0$ for all $\mathbf{x}\in\Gamma$. Since $\tilde{G}_k^{qper,p}$ satisfies the outgoing condition for $z\to\infty$, u does also, so by the uniqueness of the outgoing Dirichlet boundary-value problem for the region "above" Γ ($z > f(x,y)$), we have $u(\mathbf{x}) = 0$ for all $\mathbf{x}$ in this region. We show next that this implies the vanishing of all the Fourier coefficients $c_{j\ell}$ of $u(\mathbf{x})$ for $z > z_+$.

First consider $(j,\ell)\notin U$. The factor

$$\frac{1}{\gamma_{j\ell}}\left(1-e^{i\gamma_{j\ell}d}\right)^p + b_{j\ell} \tag{37}$$

multiplying $c_{j\ell}$ in (37) is analytic in d and therefore vanishes only on a set of values of d whose intersection with any interval $[0,d_0]$ is finite. These values of d depend on $b_{j\ell}$. But the $b_{j\ell}$ take on only a finite number of values since they vanish for all but a finite number of pairs (j,ℓ). Thus in any interval $[0,d_0]$, the factors (37) are nonzero for all (j,ℓ) except at only a finite number of values. Denote this set of values by D. By choosing $d\notin D$, one obtains $c_{j\ell}=0$ for $(j,\ell)\notin U$. Consider now $(j,\ell)\in U$. Setting $u_{j\ell}(z)$ to zero and assuming $d\neq b_{j\ell}$ for $p=1$ gives $c_{j\ell}=0$ ($b_{j\ell}$ is assumed to be nonzero).

One deduces that

$$u^0_{j\ell}(z) = \begin{cases} 0\,, & (j,\ell)\notin U\,,\\ -ic'_{j\ell}+c''_{j\ell}\,, & (j,\ell)\in U\,.\end{cases}$$

Therefore $u^0(\mathbf{x}) \;=\; \sum_{(j,\ell)\in U}(-ic'_{j\ell} + c''_{j\ell})\,e^{i(\alpha_j x+\beta_\ell y)}$ for $z > z_+$. The field $u^0(\mathbf{x})$ satisfies the Helmholtz equation for $\mathbf{x}\notin\Gamma$, and $u^0(\mathbf{x})$ is independent of z for $z>z_+$. Because of the real-analyticity of $u^0(\mathbf{x})$ for $\mathbf{x}\notin\Gamma$, $u^0(\mathbf{x})$ is independent of z above Γ, that is, for $z > f(x,y)$, and one obtains

$$u^0(\mathbf{x}) \;=\; \sum_{(j,\ell)\in U} (-ic'_{j\ell}+c''_{j\ell})\, e^{i(\alpha_j x+\beta_\ell y)} \qquad \text{for } z\geq f(x,y)\,. \tag{38}$$

Below Γ, u^0 has a Fourier expansion

$$u^0(\mathbf{x}) = \sum_{j,\ell\in\mathbb{Z}} u^{0-}_{j\ell}\, e^{i(\alpha_j x+\beta_\ell y)} \qquad (z<z_-).$$

For $(j,\ell)\in U$, the coefficients $u^{0-}_{j\ell}(z)$ are minus those for $z>z_+$ because of the absolute value $|z-z'|$ in $B(\mathbf{x}-\mathbf{x}')$:

$$u^{0-}_{j\ell}(z) = -u^{0+}_{j\ell}(z) = -i(c_{j\ell}z-c'_{j\ell})-c''_{j\ell}\,.$$

(There is no such relation for $(j\ell)\notin U$.) Since $c_{j\ell}=0$, one obtains

$$u^{0-}_{j\ell}(z) = ic'_{j\ell}-c''_{j\ell}\,.$$

Since $u^0(\mathbf{x})$ has no linear term in z for $z<z_-$, it satisfies the outgoing condition below Γ $(z<z_-)$. The field (38), if extended to all of $\mathbb{R}^3$, is a Helmholtz field that satisfies the outgoing condition for $z\to\infty$ *and* $z\to-\infty$. Thus, by subtracting if from $u^0(\mathbf{x})$, one obtains a field

$$\tilde{u}^0(\mathbf{x}) := u^0(\mathbf{x}) - \sum_{(j,\ell)\in U} (-ic'_{j\ell}+c'')e^{i(\alpha_j x+\beta_\ell y)} \qquad (\mathbf{x}\in\mathbb{R}^3)$$

that is outgoing and that vanishes for $z>f(x,y)$. The jump conditions of the single- and double-layer potentials imply that the limits of $\tilde{u}^0(\mathbf{x})$ and its normal derivative from below Γ are

$$\tilde{u}^0(x,y,f(x,y)-0) \;=\; -\xi\,\phi(x,y,f(x,y))\,, \tag{39}$$

$$\frac{\partial\tilde{u}^0}{\partial\mathbf{n}(\mathbf{x})}(x,y,f(x,y)-0) \;=\; i\eta\,\phi(x,y,f(x,y))\,. \tag{40}$$

So $\tilde{u}^0(\mathbf{x})$ for $z\leq f(x,y)$ satisfies a homogeneous impedance boundary condition on Γ,

$$\frac{\partial\tilde{u}^0}{\partial\mathbf{n}(\mathbf{x})}(x,y,f(x,y)) + \frac{i\eta}{\xi}\tilde{u}^0(x,y,f(x,y)) = 0.$$

Since $\tilde{u}^0$ is outgoing in Γ^-, Lemma 2.1 tells us that $\tilde{u}^0(\mathbf{x})=0$ below Γ. Because of (39), one concludes that $\phi(\mathbf{x})=0$ for all $\mathbf{x}\in\Gamma$. $\square$

4.3 Convergence of the modified Green function at Wood frequencies

The proof of super-algebraic convergence of the truncated Green function as $a\to\infty$ is obstructed only by the existence of a finite number of points (j,ℓ) of the dual lattice that satisfy the Wood, or cutoff, condition

$$k^2 = \left(\alpha+\frac{2\pi j}{d_1}\right)^2 + \left(\beta+\frac{2\pi\ell}{d_2}\right)^2 .$$

This is manifest in the vanishing of ∇g in the proof of Theorem 3.1 for the lattice point (j,ℓ), which prohibits integration by parts. It is precisely these terms in the sum over the dual lattice that dominate the sum as $a\to\infty$. In Theorem 4.3, it is proved that the truncated spatial lattice sum for the p^{th}-order linear combination of Green functions (31) converges at an algebraic rate of $1/a^{\lceil p/2\rceil-1/2}$.

In preparation for proving this, let us examine the individual terms of (31). Each term is of the form

$$h(\rho,\epsilon,\hat{\epsilon}) := \sum_{q=0}^{p} a_{pq}\, g(\rho,\epsilon+q\hat{\epsilon})\,; \qquad g(\rho,\epsilon) := \frac{e^{ik\rho\sqrt{1+\epsilon^2}}}{\rho\sqrt{1+\epsilon^2}}\,,$$

times the phasor $e^{i(\alpha m d_1+\beta n d_2)}$, in which

$$\begin{aligned} &\rho=\rho_{mn}=\sqrt{(x-\hat{x}+md_1)^2+(y-\hat{y}+nd_2)^2}\,,\\ &\epsilon=(z-z')/\rho\,, \quad \hat{\epsilon}=d/\rho\,. \end{aligned}$$

The crucial point is that the p^{th} difference $h(\rho,\epsilon,\hat{\epsilon})$ behaves as a specific power of $1/\rho$, given in Lemma 4.2, as (m,n), or equivalently ρ, becomes large.

Because of (32) and the analyticity of $h(\rho,\epsilon,\hat{\epsilon})$, we obtain, for some constants C_d and C_d',

$$h(\rho,\epsilon,\hat{\epsilon}) \;=\; C_p\,\hat{\epsilon}^p\,\frac{\partial^p g}{\partial\epsilon^p}(\rho,\epsilon)+C_p'\,\hat{\epsilon}^{p+1} g_p(\rho,\epsilon,\hat{\epsilon}),$$

in which g_p is analytic and

$$|g_p(\rho,\epsilon,\hat{\epsilon})| \;<\; \sup_{|\eta|\le p\hat{\epsilon}}\left|\frac{\partial^{p+1}g}{\partial\epsilon^{p+1}}(\rho,\epsilon+\eta)\right|\,.$$

Using the relations $\epsilon=(z-z')/\rho$ and $\hat{\epsilon}=d/\rho$,

$$h\left(\rho,\,(z-z')/\rho,\,d/\rho\right) \;=\; C_p\left(\frac{d}{\rho}\right)^p \frac{\partial^p g}{\partial\epsilon^p}(\rho,(z-z')/\rho)+C_p'\left(\frac{d}{\rho}\right)^{p+1} g_p\big(\rho,(z-z')/\rho,d/\rho\big)\,. \tag{41}$$

In view of the Lemma 4.2 below,

$$h\big(\rho,\,(z-z')/\rho,\,d/\rho\big) \;=\; \mathcal{O}\left(\frac{1}{\rho^{\lceil\frac{p}{2}\rceil+1}}\right) \qquad (\rho\to\infty), \tag{42}$$

where the constant in the $\mathcal{O}$-term depends on z, $\hat{z}$, d, and p and can be taken to be fixed if d and p are given and $(z,\hat{z})$ is contained in a bounded set of $\mathbb{R}^2$.

Lemma 4.2.

$$\frac{1}{\rho^p}\frac{\partial^p g}{\partial\epsilon^p}(\rho,\epsilon)=\mathcal{O}\left(\frac{1}{\rho^{\lceil\frac{p}{2}\rceil+1}}\right) \qquad (\rho\to\infty), \tag{43}$$

in which $\lceil\cdot\rceil$ denotes the ceiling. Big-O cannot be replaced by little-o, and the constant C in $\mathcal{O}(\rho^b)\le C\rho^b$ $(b=\lceil\frac{p}{2}\rceil+1)$ depends analytically on ϵ.

Proof. The p^{th} derivative $\frac{\partial^p g}{\partial\epsilon^p}$ of g with respect to ϵ is a sum of terms of the form

$$C\,\frac{\epsilon^m(ik\rho)^n}{\sqrt{1+\epsilon^2}^{\,\ell}}\,\frac{e^{ik\rho\sqrt{1+\epsilon^2}}}{\rho} \tag{44}$$

for various values of (C, m, n, ℓ), with $C, m \in \mathbb{Z}$ and $(n, \ell) \in \mathbb{N}_0$. Define, for all integers m and nonnegative integers n and ℓ,

$$T(m,n,\ell) = \frac{\epsilon^m (ik\rho)^n}{\sqrt{1+\epsilon^2}^{\ell}} \quad \text{for } m,n,\ell \geq 0,$$
$$T(m,n,\ell) = 0 \quad \text{for } m < 0.$$

The terms $T(m,n,\ell)$ in the composition of $\frac{\partial^p g}{\partial \epsilon^p}$ can be computed recursively using the rules

$$g(\rho,\epsilon) = T(0,0,1)\frac{e^{ik\rho\sqrt{1+\epsilon^2}}}{\rho},$$
$$\frac{\partial}{\partial\epsilon}\left(T(m,n,\ell)\frac{e^{ik\rho\sqrt{1+\epsilon^2}}}{\rho}\right) = \left(-\ell f^- T(m,n,\ell) + f^0 T(m,n,\ell) + m f^+(m,n,\ell)\right)\frac{e^{ik\rho\sqrt{1+\epsilon^2}}}{\rho} \quad (m \geq 0),$$
$$\frac{\partial}{\partial\epsilon}\left(T(m,n,\ell)\frac{e^{ik\rho\sqrt{1+\epsilon^2}}}{\rho}\right) = 0 \quad (m < 0),$$

in which the operators $f^{-,0,+}$ are defined by

$$f^- T(m,n,\ell) = T(m+1, n, \ell+2),$$
$$f^0 T(m,n,\ell) = T(m+1, n+1, \ell+1),$$
$$f^+ T(m,n,\ell) = T(m-1, n, \ell).$$

From the definition $\epsilon = z/\rho$, one finds that

$$T(m,n,\ell) \sim z^m (ik)^n \rho^{n-m} \quad (\rho \to \infty) \quad \text{for } m \geq 0.$$

Define the order Q of $T(m,n,\ell)$ by

$$Q(T(m,n,\ell)) = n - m \quad (m \geq 0),$$
$$Q(T(m,n,\ell)) = -\infty \quad (m < 0).$$

Notice that f^+, f^-, and f^0 respectively increase, leave fixed, and decrease the order $Q(T)$ and that f^- decreases the power of ϵ by one while f^0 and f^+ increase it by one.

The derivative $\frac{\partial^p g}{\partial \epsilon^p}$ is a sum of 3^p terms of the form $CT(m,n,\ell)$ (pairs of these could have the same (m,n,ℓ) and some are zero), obtained by applying a sequence of p operations from the set $\{f^-, f^0, f^+\}$ to the root expression $T(0,0,1)$.

Let $CT(m,n,\ell)$ be a term of $\frac{\partial^p g}{\partial \epsilon^p}$, associated with a sequence of p operations f_i, $i = 1,\ldots,p$. In order that $m \geq 0$, no more than half of the f_i may be equal to f^+. Thus the order of $T(m,n,\ell)$ is at most $Q_+ = p/2$ if p is even and $Q_+ = (p-1)/2$ if p is odd.

To see that there is a nonzero term $T(m,n,\ell)$ with order Q_+, take $T(m,n,\ell) = (f^+)^{\frac{p}{2}}(f^0)^{\frac{p}{2}}T(0,0,1)$ if p is even and $T(m,n,\ell) = (f^+)^{\frac{p-1}{2}}(f^0)^{\frac{p+1}{2}}T(0,0,1)$ if p is odd.

If $C < 0$ in a term $CT(m,n,\ell)$ in the composition of $\frac{\partial^p g}{\partial \epsilon^p}$, then, by the recursion rule, one of the operations f_i must be equal to f^-. Since at most half of the f_i are equal to f^+, we have $Q(T) \leq Q_+ - 1$. Thus all of the T of order Q_+ have nonzero coefficients, one of which is positive, and we infer that their sum is nonzero.

Finally, taking into account the factor of $1/\rho$ in (44), the statement follows. ∎

Now we are able to prove the algebraic convergence of the lattice sum for $G_k^{qper,p}(\mathbf{x})$.

Theorem 4.3 (Modified Green function for all frequencies; algebraic convergence)**.** *Let $\chi(s,t)$ be a smooth truncation function equal to 1 for $s^2+t^2<A^2>0$ and equal to 0 for $s^2+t^2>B^2$. For all triples (k,α,β), and integers $p\geq 1$, the sums*

$$G_k^{p,a}(\mathbf{x}) = \frac{1}{4\pi}\sum_{m,n\in\mathbb{Z}} e^{-i(\alpha m d_1+\beta n d_2)}\sum_{q=0}^{p} a_{pq}\frac{e^{ikr_{mn}^{pq}}}{r_{mn}^{pq}}\,\chi(\tfrac{md_1}{a},\tfrac{nd_2}{a})\ , \tag{45}$$

in which, $r_{mn}^{pq} = \sqrt{(x+md_1)^2+(y+nd_2)^2+(z+qd)^2}$, converge to a radiating quasi-periodic modified Green function $G_k^{qper,p}(\mathbf{x})$, that is,

$$\nabla_{\mathbf{x}}^2 G_k^{qper,p}(\mathbf{x}) + k^2 G_k^{qper,p}(\mathbf{x}) \;=\; -\sum_{m,n\in\mathbb{Z}}\sum_{q=0}^{p}\delta(\mathbf{x}+(md_1,nd_2,qd))e^{i(\alpha m d_1+\beta n d_2)}\,,$$

and $G_k^{qper,p}(\mathbf{x}+(md_1,nd_2,0)) = G_k^{qper,p}(\mathbf{x})e^{i(\alpha m d_1+\beta n d_2)}$. Specifically, for each bounded set $K\in\mathbb{R}^3$, there exist constants C^p for $p\geq 1$ such that

$$\left|G_k^{p,a}(\mathbf{x}) - G_k^{qper,p}(\mathbf{x})\right| < \frac{C^p}{a^{\lceil p/2\rceil-1/2}}$$

if a is sufficiently large and $\mathbf{x}\in K$, $(x,y,z)\notin d_1\mathbb{Z}\times d_2\mathbb{Z}\times\{0\}$.

Proof. Set $\nu=\lceil p/2\rceil+1$. The sum (45) can be written as

$$G_k^{p,a}(\mathbf{x}) \;=\; \frac{1}{4\pi}\sum_{m,n\in\mathbb{Z}} h(\rho_{mn}, z/\rho_{mn}, d/\rho_{mn})e^{-i(\alpha m d_1+\beta n d_2)}\chi(\tfrac{md_1}{a},\tfrac{nd_2}{a})\,.$$

in which $\rho_{mn}=\sqrt{(x+md_1)^2+(y+nd_2)^2}$. In view of (42), the terms of this sum can be written as

$$\frac{1}{4\pi}h\left(\rho_{mn}, z/\rho_{mn}, d/\rho_{mn}\right) = \frac{1}{\left((md_1)^2+(nd_2)^2\right)^{\nu/2}}H(\mathbf{x};md_1,nd_2)$$

for some function H such that there are constants C and M for which $H(\mathbf{x};md_1,nd_2)<C$ as long as $(\mathbf{x})$ is restricted to a bounded region K in $\mathbb{R}^3$ and $(m,n)\in\mathbb{Z}^2$ is restricted by $|(md_1,nd_2)|>M$.

For $p\geq 1$, apply the Poisson Summation Formula to $G^{p,b}-G^{p,a}$, with $a<b$:

$$\begin{aligned}
&G_k^{p,b}(\mathbf{x}) - G_k^{p,a}(\mathbf{x})\\
&\quad= \sum_{m,n\in\mathbb{Z}}\frac{H(\mathbf{x};md_1,nd_2)}{((md_1)^2+(nd_2)^2)^{\nu/2}}\left(\chi(\tfrac{md_1}{a},\tfrac{nd_2}{a})-\chi(\tfrac{md_1}{b},\tfrac{nd_2}{b})\right)e^{-i(\alpha m d_1+\beta n d_2)}\\
&\quad= \frac{1}{d_1d_2}\sum_{j,\ell\in\mathbb{Z}}\iint_{\mathbb{R}^2}\frac{H(\mathbf{x};\hat{x},\hat{y})}{(\hat{x}^2+\hat{y}^2)^{\nu/2}}\left(\chi(\tfrac{\hat{x}}{a},\tfrac{\hat{y}}{a})-\chi(\tfrac{\hat{x}}{b},\tfrac{\hat{y}}{b})\right)e^{-i\left((\alpha+\frac{2\pi}{d_1}j)\hat{x}+(\beta+\frac{2\pi}{d_2}\ell)\hat{y}\right)}d\hat{x}d\hat{y}\\
&\quad= \frac{1}{d_1d_2}\sum_{j,\ell\in\mathbb{Z}}I_{j\ell}^{ab},
\end{aligned}$$

in which $I_{j\ell}^{ab}$ denotes the Fourier integral in the sum. For a given lattice point (j,ℓ), put $\langle\alpha+\frac{2\pi}{d_1}j,\beta+\frac{2\pi}{d_2}\ell\rangle = \xi_{j\ell}\langle\cos\gamma_{j\ell},\sin\gamma_{j\ell}\rangle$. By the argument of the proof of Theorem 3.1, one shows that the dual-lattice sum of the $I_{j\ell}^{ab}$, excluding the finite set of pairs (j,ℓ) for which $k=\xi_{j\ell}$ (equivalently

$\gamma_{j\ell} = 0$), is bounded by a multiple of any power of $1/a$, independently of b and of $\mathbf{x} \in K$. (One simply has a finite linear combination over q of dual-lattice sums of the type treated in Step 1 of that proof.) In particular, we have

$$\sum_{\substack{j,\ell \in \mathbb{Z} \\ |k| \neq |\xi|}} I_{j\ell}^{ab} \;<\; \frac{C}{a^{\nu-3/2}}\,.$$

As $k > 0$, we now assume $\xi_{j\ell} \neq 0$ and prove algebraic rate of convergence of $I_{j\ell}^{ab}$ as $a, b \to \infty$, for the finite set of pairs (j,ℓ) such that $k = \xi_{j\ell}$. Under the change of coordinates $(\hat{x}, \hat{y}) = ra(\cos\theta, \sin\theta)$, the integral becomes

$$I_{j\ell}^{ab} \;=\; \frac{1}{a^{\nu-2}} \int_A^\infty \frac{1}{r^{\nu-1}} \int_0^{2\pi} H\big(\mathbf{x}; ra\cos\theta, ra\sin\theta\big)\phi_{a,b}(r\cos\theta, r\sin\theta) e^{-iar\xi\cos(\theta-\gamma)}\, d\theta dr\,,$$

in which the function

$$\phi_{a,b}(s,t) \;=\; \chi(\tfrac{a}{b}s, \tfrac{a}{b}t) - \chi(s,t)$$

is smooth and compactly supported and tends pointwise up to $1 - \chi(s,t)$. The phase of the inner integral has two stationary points: $\theta = \gamma$ and $\theta = \gamma + \pi$; and the method of stationary phase yields

$$I_{j\ell}^{ab} \;=\; \frac{1}{a^{\nu-3/2}} \sqrt{\frac{2\pi}{\xi}} \int_A^\infty \frac{1}{r^{\nu-1/2}} \times \\ \sum_{\pm} H\big(\mathbf{x}, \pm ra\cos\gamma, \pm ra\sin\gamma\big)\phi_{a,b}(\pm r\cos\gamma, \pm r\sin\gamma) e^{\mp i(ar\xi - \pi/4)} \cdot \mathcal{O}(1)\, dr,$$

in which the order-1 function $\mathcal{O}(1)$ is bounded by a constant for a sufficiently large and $r > A$. As long as $\nu > 3/2$ (*i.e.*, $p \geq 1$), $aA > M$, and $\mathbf{x} \in K$, the integral in r is finite and bounded independently of a and $b > a$. Thus we obtain

$$\left| I_{j\ell}^{ab} \right| \;<\; \frac{C'}{a^{\nu-3/2}} = \frac{C'}{a^{\lceil p/2 \rceil - 1/2}}\,,$$

and thus a constant C^p such that $|G_k^{p,b}(\mathbf{x}) - G_k^{p,a}(\mathbf{x})| \;<\; C^p/a^{\lceil p/2 \rceil - 1/2}$. We infer that $G_k^{p,a}(\mathbf{x})$ converges to a function $G_k^p(\mathbf{x})$ at the algebraic rate stated in the theorem:

$$\big| G_k^p(\mathbf{x}) - G_k^{p,a}(\mathbf{x}) \big| \;<\; \frac{C^p}{a^{\lceil p/2 \rceil - 1/2}}$$

for a sufficiently large and $\mathbf{x} \in K$.

The proof that $G_k^p(\mathbf{x})$ is a radiating quasi-periodic Green function follows arguments analogous to Steps 2–4 in the proof of Theorem 3.1. ■

5 High-order evaluation of the boundary-layer potentials with quasi-periodic Green functions

In order to obtain high-order discretizations of the integral operators that involve quasi-periodic Green functions we use our previously developed strategy based on non-overlapping Chebyshev

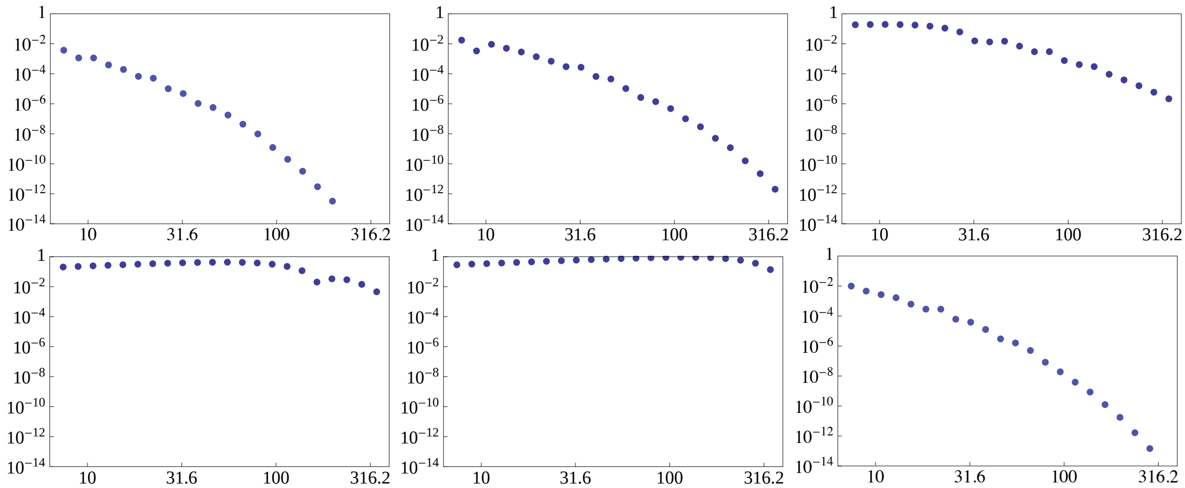

Figure 1: The error in the approximation of the quasi-periodic Green function by multiplying the lattice sum by a smooth truncation function $\chi((m+x)/a)\chi((n+y)/a)$, in which $\chi(s) = \exp(2e^{1/(1-x)}/(x-2))$. The plots show $\max_{(x,y,z)\in K} |G_{i+1} - G_i|$ as a function of a_i on a *log-log* scale, in which a truncated lattice sum G_i is computed for $a = a_i = 1.2^i$, $\hat{\mathbf{x}} = (\hat{x}, \hat{y}, \hat{z}) = (0, 0, 1)$ and (x, y, z) on a grid K of evenly spaced points in $[0, 0.6] \times [0, 0.6] \times [0.6, 1.4]$, excluding $\hat{\mathbf{x}} = \mathbf{x}$. The period is 1, the Bloch wavevector is $(\kappa_1 = 0, \kappa_2 = 0)$, and the frequencies are $k = 0.4, 0.8, 0.95$ (first row) and $k = 0.99, 2.24, 2.5$ (second row). Both $k = 1.0$ and $k \approx 2.23607$ are Wood frequencies, at which convergence is not available.

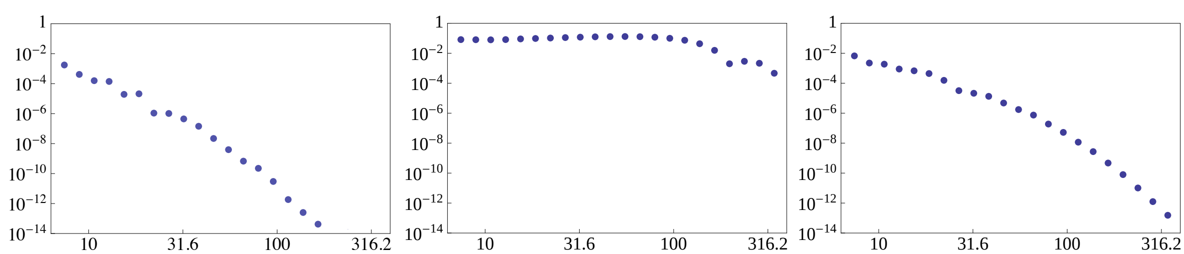

Figure 2: These plots are similar to those in Fig. 1 except that the Bloch wavevector is $(\kappa_1 = 0.4, \kappa_2 = -0.3)$, and the frequencies are $k = 0.3, 0.93, 1.1$. There is a Wood frequency at ~ 0.921954.

patches. Our Nyström discretization produces high-order quadratures for the evaluation of integral operators of the kind

$$(\mathcal{I}\mu)(\mathbf{x}) = \int_S \left(\frac{\partial G^a(\mathbf{x};\mathbf{x}')}{\partial \mathbf{n}(\mathbf{x}')} + i\tau G^a(\mathbf{x};\mathbf{x}')\right)\mu(\mathbf{x}')ds(\mathbf{x}'),\ \mathbf{x}\in S$$

where μ is a density defined on the surface S and

$$\begin{aligned} G^a(\mathbf{x};\mathbf{x}') &= \frac{1}{4\pi}\sum_{m,n\in\mathbb{Z}} \frac{e^{ik\left((x_1-x_1'+md_1)^2+(x_2-x_2'+nd_2)^2+(x_3-x_3')^2\right)^{1/2}}}{\left((x_1-x_1'+md_1)^2+(x_2-x_2'+nd_2)^2+(x_3-x_3')^2\right)^{1/2}} \\ &\times\ e^{-i(\alpha md_1+\beta nd_2)}e^{i\alpha(x_1'-x_1)}e^{i\beta(x_2'-x_2)}\,\chi(\tfrac{md_1}{a},\tfrac{nd_2}{a}). \end{aligned}$$

We note that the term corresponding to $(m,n)=(0,0)$ in the definition of the function $G^a(\mathbf{x};\mathbf{x}')$ coincides with the free-space Green function $G_k(|\mathbf{x}-\mathbf{x}'|)$ which is singular when $\mathbf{x}=\mathbf{x}'$, whereas all the other terms in the summation involved in the definition of $G^a(\mathbf{x};\mathbf{x}')$ are smooth. Our integration algorithm assumes that the integration surface S is tiled by polygonal regions that can be discretized with high-order accuracy by means of cosine transforms and Chebyshev approximations. Our high-order integration algorithm consists of two main stages corresponding to the treatment of well-separated interactions (given a target point $\mathbf{x}$, that is the contribution to the integral of (i) the terms $G_k(|\mathbf{x}-\mathbf{x}'|)$ for all integration points $\mathbf{x}'$ well-separated from $\mathbf{x}$ and (ii) the terms in the definition of $G^a(\mathbf{x};\mathbf{x}')$ corresponding to all pairs $(m,n)\neq(0,0)$ and all integration points $\mathbf{x}'$) and adjacent/singular and near-singular interactions. The first stage of our algorithm consists of (a) Singular integration, based on polar coordinate transformations, which are used around each observation point in a given patch using floating partitions of unity; and (b) near singular integration: for smooth portions of the scattering surface and for observation points close to but *outside* the integration patch, we perform polar integration centered at the observation point. On the other hand, in the second stage of our algorithm, for each integration patch, we treat the interactions of the first type by means of Clenshaw-Curtis-type integrations. Furthermore, the far-away interactions are accelerated by use of equivalent sources placed on Cartesian grids and 3D sparse FFT convolutions that generalizes the approach introduced in [5] to the case of evaluating far-away interactions via G^a which we describe next.

The first step of the acceleration method consists of partitioning a cube C of size A circumscribing the scatterer into L^3 identical cubic cells c_i of size adjusted (in the sense of small enough) so that they do not admit either inner acoustic resonances – eigenfunctions of the Laplacean with Dirichlet boundary conditions. The main idea of the acceleration algorithm is to seek to substitute the surface "true" sources which correspond to the discretization points contained in a certain cube c_i by acoustic periodic "equivalent sources" on the faces of c_i in a manner such that the acoustic fields generated by the c_i-equivalent sources approximate to high order accuracy the fields produced by the true c_i sources at all points in space non-adjacent to c_i. The precise concept of adjacency [5] results from requiring that the approximation corresponding to a given cell c_i be valid within exponentially small errors outside the concentric cube $\mathcal{S}_i$ of triple size. At the heart of this method lies the use of equivalent sources which consist of acoustic monopoles and dipoles placed on three independent sets Π^l_{ac}, each one parallel to $x_l=0$. For a fixed value $l=1,2,3$, we associate to an acoustic field u and each cell c_i-equivalent sources, acoustic monopoles $\xi^{(m)l}_{i,j}\ G^{L,per}_k(\mathbf{x}-\mathbf{x}^l_{i,j})$ and dipoles $\xi^{(d)l}_{i,j}\ \partial G^{L,per}_k(\mathbf{x}-\mathbf{x}^l_{i,j})/\partial x_l$ placed at points $\mathbf{x}^l_{i,j}, l=1,\cdots,M^{equiv}$ contained within certain subsets Π^l_i which lie within the union of two circular domains concentric with and circumscribing the faces of c_i, their radius chosen according to the prescriptions in [5]. The fields $\psi^{c_i,true}$ radiated by the c_i-true sources are approximated themselves by fields $\psi^{c_i,eq}$ radiated by the c_i-equivalent sources

$$\psi^{c_i,eq}(\mathbf{x}) = \sum_{j=1}^{\frac{1}{2}M^{equiv}} \left(\xi_{i,j}^{(m)l}\ G^a(\mathbf{x}, \mathbf{x}_{i,j}^l) + \xi_{i,j}^{(d)l} \frac{\partial G^a(\mathbf{x}, \mathbf{x}_{i,j}^{(d)l})}{\partial x_l} \right). \tag{46}$$

The parameters n_t, M^{equiv} and the unknown monopole and dipole intensities in (46) are chosen so that the truncated spherical wave expansions of order n_t for $\psi^{c_i,true}$ and $\psi^{c_i,eq}$ differ in no more than $\mathcal{O}(\epsilon)$ outside $\mathcal{S}_i$. Based on considerations on spherical harmonics, it was required in [5] that $M^{equiv} \gtrsim n_t^2$ equivalent sources are used for each acoustic component and the the intensities are chosen such that to minimize in the mean-square norm the differences $(\psi^{c_i,eq}(\mathbf{x}) - \psi^{c_i,true}(\mathbf{x}))$ as $\mathbf{x}$ varies over a number n^{coll} collocation points on $\partial\mathcal{S}_i$. Hence, the intensities in (46) are obtained in practice as the least-squares solution of three overdetermined linear systems $\mathbf{A}\xi = \mathbf{b}$ where $\mathbf{A}$ are $n^{coll} \times M^{equiv}$ matrices. This strategy leads to a total computational cost of $\mathcal{O}(4a^2N^{4/3}\log N + n_{iter}N^{4/3}\log N)$ to solve integral equations based on boundary layer potentials involving G^a, where N is the number of discretization points and n_{iter} is the number of iterations required by the linear algebra iterative solver (e.g. GMRES) to reach a desired small tolerance.

5.1 Diffraction gratings

We present in this section a version of the high-order integration procedure introduced in [5]. We can reformulate the quasi-periodic scattering integral equation (19) in a manner that involves only *periodic* quantities. To that end, we use the fact that if the solution ϕ of the integral equation (19) is (α, β) quasi-periodic, then the quantity

$$\phi_{per}(x, y) = e^{-i\alpha x} e^{-i\beta y} \phi(x, y)$$

is actually (d_1, d_2) periodic, which allows one to express the integral equation (19) in the form

$$\begin{aligned} \frac{\xi\phi_{per}(\mathbf{x})}{2} \quad &+ \quad \int_{\Gamma^{per}} \left(\xi \frac{\partial G_k^{per}(\mathbf{x}, \mathbf{x}')}{\partial \mathbf{n}(\mathbf{x}')} + i\eta G_k^{per}(\mathbf{x}, \mathbf{x}') \right) \phi_{per}(\mathbf{x}') ds(\mathbf{x}') \\ &= \quad -e^{ikd_3 f(x,y)},\ (x, y),\ (x', y') \in [0, d_1] \times [0, d_2]. \end{aligned} \tag{47}$$

where the (d_1, d_2) *periodic* Green function G_k^{per} is defined as

$$G_k^{per}(\mathbf{x}, \mathbf{x}') = G_k^{per}(\mathbf{x} - \mathbf{x}') = G_k^{qper}(\mathbf{x}, \mathbf{x}') e^{i\alpha(x'-x)} e^{i\beta(y'-y)}. \tag{48}$$

Similarly, by the same phase-extraction procedure, the representation in equation (35) using the modified Green function $\tilde{G}_k^{qper,p}$ can be re-expressed in terms of periodic quantities $\tilde{G}_k^{per,p}$.

In the periodic formulation of the various integral equation formulations introduced in this paper, we have to deal with evaluations of double-layer potential operators of the kind

$$(\mathcal{K}\phi)(\mathbf{x}) = \int_{\Gamma_{per}} \frac{\partial G_k^{per}(\mathbf{x} - \mathbf{x}')}{\partial \mathbf{n}(\mathbf{x}')} \phi(\mathbf{x}') ds(\mathbf{x}'), \tag{49}$$

and single-layer potential operators of the kind

$$(\mathcal{S}\phi)(\mathbf{x}) = \int_{\Gamma_{per}} G_k^{per}(\mathbf{x} - \mathbf{x}') \phi(\mathbf{x}') ds(\mathbf{x}'), \tag{50}$$

where the periodic Green function G_k^{per} has the same singularity as the free-space Green function G_k when $\mathbf{x} = \mathbf{x}'$ and ϕ is a periodic and smooth density. If we assume a parametrization of Γ_{per} in the form $\Gamma_{per} = \{(x, y, f(x, y)) : 0 \le x < d_1 \quad 0 \le y < d_2\}$ such that $\mathbf{x} = (x, y, f(x, y))$ and $\mathbf{x}' = (x', y', f(x', y'))$, we apply the above phase extraction to the function $G_k^a(x, y; x', y')$ defined in equation (24) to obtain the function $G^a(x, y; x', y')$ defined as

$$\begin{aligned} G^a(x,y;x',y') &= \frac{1}{4\pi}\sum_{m,n\in\mathbb{Z}} \frac{e^{ik\left((x-x'+md_1)^2+(y-y'+nd_2)^2+(f(x,y)-f(x',y'))^2\right)^{1/2}}}{\left((x-x'+md_1)^2+(y-y'+nd_2)^2+(f(x,y)-f(x',y'))^2\right)^{1/2}} \\ &\times \; e^{-i(\alpha m d_1+\beta n d_2)} e^{i\alpha(x'-x)} e^{i\beta(y'-y)}\,\chi\!\left(\tfrac{md_1}{a},\tfrac{nd_2}{a}\right). \end{aligned}$$

Away from Wood frequencies, the functions $G^a(x, y; x', y')$ converge super-algebraically to the function $G(x, y; x', y')$ as $a \to \infty$ for all $(x, y),\ (x', y') \in [0, d_1) \times [0, d_2)$. We use the function G^a to define operators $\mathcal{K}^a$ and $\mathcal{S}^a$ in parametric form in the following manner,

$$\begin{aligned} (\mathcal{K}^a\phi)(x,y) &= \int_{x-d_1/2}^{x+d_1/2}\int_{y-d_2/2}^{y+d_2/2} \nabla G^a(x,y;x',y')\cdot(-f_{x'},-f_{y'},1)\phi(x',y')dx'dy'\,, \\ (\mathcal{S}^a\phi)(x,y) &= \int_{x-d_1/2}^{x+d_1/2}\int_{y-d_2/2}^{y+d_2/2} G^a(x,y;x',y')\phi(x',y')g(x',y')dx'dy' \end{aligned} \tag{51}$$

where $\nabla G^a(x, y; x', y') = \nabla_{\mathbf{x}'} G^a(\mathbf{x} - \mathbf{x}')$ and $g(x', y') = (f_{x'}^2 + f_{y'}^2 + 1)^{1/2}$ is the surface element.

We have that for any *target* point $(x, y) \in [0, d_1) \times [0, d_2)$, all the terms in the definition of G^a corresponding to $(m, n) \neq (0, 0)$ are smooth for all *integration* points (x', y'), and that the terms corresponding to $(m, n) = (0, 0)$ coincide with the free-space Green function $G_k(x, y; x', y')$, which is singular when the target and integration points coincide. Specifically, we can write

$$\begin{aligned} G^a(x,y;x',y') &= G_{SL}^{sing}(x,y;x',y') + G_{SL}^{a,smooth}(x,y;x',y') \\ \nabla G^a(x,y;x',y')\cdot(-f_{x'},-f_{y'},1) &= G_{DL}^{sing}(x,y;x',y') + G_{DL}^{a,smooth}(x,y;x',y') \end{aligned}$$

where

$$\begin{aligned} G_{SL}^{sing}(x,y;x',y') &= \frac{\cos k\|\mathbf{R}\|}{4\pi\|\mathbf{R}\|} e^{i\alpha(x'-x)} e^{i\beta(y'-y)} \\ G_{DL}^{sing}(x,y;x',y') &= \left(\frac{\cos k\|\mathbf{R}\|}{\|\mathbf{R}\|} + k\sin k\|\mathbf{R}\|\right)\frac{\mathbf{R}\cdot(-f_{x'},-f_{y'},1)}{4\pi\|\mathbf{R}\|^2} e^{i\alpha(x'-x)} e^{i\beta(y'-y)} \end{aligned}$$

and

$$
\begin{aligned}
G_{SL}^{a,smooth}(x,y;x',y') &= i\frac{\sin k\|\mathbf{R}\|}{4\pi\|\mathbf{R}\|}e^{i\alpha(x'-x)}e^{i\beta(y'-y)} \\
&+ \frac{1}{4\pi}\sum_{m,n\in\mathbb{Z},(m,n)\neq(0,0)}\frac{e^{ik\|\mathbf{R}_{mn}\|}}{\|\mathbf{R}_{mn}\|} \\
&\times e^{i(\alpha md_1+\beta nd_2)}e^{i\alpha(x'-x)}e^{i\beta(y'-y)}\,\chi(\tfrac{md_1}{a},\tfrac{nd_2}{a}) \\
&= \sum_{m=-L}^{L}\sum_{n=-L}^{L}G_{mn}^{SL}(x,y;x'+md_1,y'+nd_2) \\
G_{DL}^{a,smooth}(x,y;x',y') &= i\left(\frac{\sin k\|\mathbf{R}\|}{\|\mathbf{R}\|}-k\cos k\|\mathbf{R}\|\right)\frac{\mathbf{R}\cdot(-f_{x'},-f_{y'},1)}{4\pi\|\mathbf{R}\|^2}e^{i\alpha(x'-x)}e^{i\beta(y'-y)} \\
&+ \frac{1}{4\pi}\sum_{m,n\in\mathbb{Z},(m,n)\neq(0,0)}\left(\frac{1}{\|\mathbf{R}_{mn}\|}-ik\right)e^{ik\|\mathbf{R}_{mn}\|}\frac{\mathbf{R}_{mn}\cdot(-f_{x'},-f_{y'},1)}{4\pi\|\mathbf{R}_{mn}\|^2} \\
&\times e^{-i(\alpha md_1+\beta nd_2)}e^{i\alpha(x'-x)}e^{i\beta(y'-y)}\,\chi(\tfrac{md_1}{a},\tfrac{nd_2}{a}) \\
&= \sum_{m=-L}^{L}\sum_{n=-L}^{L}G_{mn}^{DL}(x,y;x'+md_1,y'+nd_2)
\end{aligned}
$$

where $\mathbf{R}=(x,y,f(x,y))-(x',y',f(x',y'))$, $\mathbf{R}_{mn}=\mathbf{R}+md_1\mathbf{e}_1+nd_2\mathbf{e}_2$, and $L=\max\{\lceil\frac{aB}{d_1}\rceil,\lceil\frac{aB}{d_2}\rceil\}$.

We perform the *smooth* integration of products of the kernels $G_{SL}^{a,smooth}$ and $G_{DL}^{a,smooth}$ and densities ϕ with the trapezoidal method. Given that all $G_{SL}^{a,smooth}$, $G_{DL}^{a,smooth}$, and ϕ are smooth and periodic, trapezoidal integration delivers spectral accuracy. Specifically, we consider the equispaced cartesian grid consisting of N^2 points $\mathbf{x}_{pq}=(x_p,y_q)=(\frac{pd_1}{N},\frac{qd_2}{N}),\ p,q=0,\dots N$ and we sample the density ϕ at these points; let us denote by ϕ_{pq} the value of ϕ at $\mathbf{x}_{pq}$. For each point $\mathbf{x}_{pq}$, the smooth contributions of all other discretization points (i.e. sums of products of the kernels $G_{SL}^{a,smooth}(\mathbf{x}_{pq};\mathbf{x}_{rs})$, $G_{DL}^{a,smooth}(\mathbf{x}_{pq};\mathbf{x}_{rs})$, and ϕ_{rs} for all $0\le r,s<N$) can be performed by (a) using equispaced meshes centered around x_{pq} and spanning from $pd_1/N-d_1/2$ to $pd_1+d_1/2$ and of step size d_1/N in the x direction and spanning from $qd_2/N-d_2/2$ to $qd_2/N+d_2/2$ and of step size d_2/N in the y direction, respectively, (b) extending by periodicity the values $\phi_{pq},\ 0\le p,q<N$ to those grids; and (c) using the trapezoidal method to effect the integration. If we assume that N is

even, we obtain

$$\begin{aligned}
\int_{x_p-d_1/2}^{x_p+d_1/2}\int_{y_q-d_2/2}^{y_q+d_2/2} & G_{DL}^{a,smooth}(x_p,y_q;x',y')\phi(x',y')dx'dy' \\
\approx & \frac{d_1 d_2}{N^2}\sum_{r=0}^{N/2}\sum_{s=0}^{N/2}\phi_{p-r-N\lceil\frac{p-r}{N}\rceil,q-s-N\lceil\frac{q-s}{N}\rceil} \\
\times & \left(\sum_{m=-L}^{L}\sum_{n=-L}^{L}G_{mn}^{DL}(x_p,y_q;x_p-rd_1/N+md_1,y_q-sd_2/N+nd_2)\right) \\
+ & \frac{d_1 d_2}{N^2}\sum_{r=1}^{N/2-1}\sum_{s=1}^{N/2-1}\phi_{p+r-N\lceil\frac{p+r}{N}\rceil,q+s-N\lceil\frac{q+s}{N}\rceil} \\
\times & \left(\sum_{m=-L}^{L}\sum_{n=-L}^{L}G_{mn}^{DL}(x_p,y_q;x_p+rd_1/N+md_1,y_q+sd_2/N+nd_2)\right)
\end{aligned} \tag{52}$$

where for a real number x, $\lceil x\rceil$ denotes the largest integer less than or equal to x. A similar quadrature rule is applied to the case of the kernels $G_{SL}^{a,smooth}$.

On the other hand, we deal with the *singular* integration of products of the kernel G^{sing} and densities ϕ through a *floating* partition of unity $(\eta_{x,y}, 1-\eta_{x,y})$ associated with each target point (x,y) that splits up the integration in the following manner

$$\begin{aligned}
\int_{x-d_1/2}^{x+d_1/2}\int_{y-d_2/2}^{y+d_2/2} & G_{DL}^{sing}(x,y;x',y')\phi(x',y')dx'dy' \\
= & \int_{x-d_1/2}^{x+d_1/2}\int_{y-d_2/2}^{y+d_2/2} G_{DL}^{sing}(x,y;x',y')\eta_{x,y}(x',y')\phi(x',y')dx'dy' \\
+ & \int_{x-d_1/2}^{x+d_1/2}\int_{y-d_2/2}^{y+d_2/2} G_{DL}^{sing}(x,y;x',y')(1-\eta_{x,y}(x',y'))\phi(x',y')dx'dy'
\end{aligned} \tag{53}$$

and similarly for integrations that involve the kernels G_{SL}^{sing}. Here the smooth, compactly supported Wood function $\eta_{x,y}$ is chosen such that $\eta_{x,y}(x',y')=1$ for $\|(x,y)-(x',y')\|<r_0$ and $\eta_{x,y}$ vanishes for $\|(x,y)-(x',y')\|\geq r_1$. We require that $4r_1\leq(d_1^2+d_2^2)^{1/2}$. The effect of the splitting (53) is to localize the singular integrand in a neighborhood of the point of singularity via the Wood $\eta_{x,y}$, while the other term contains the smooth and periodic factor $1-\eta_{x,y}$, which, together with the fact that the additional factors involved are smooth throughout its domain of integration, allows again for their evaluations by means of the trapezoidal rule. On the other hand, the localized singular integrand term will be evaluated through a simplified version of the high-order singular integrator introduced in [5] to the current context, a task that we will undertake next.

The high-order singular integrator that we use in the evaluation of generic integrals of the type

$$\begin{aligned}
J(x,y) &= \int_{x-d_1/2}^{x+d_1/2}\int_{y-d_2/2}^{y+d_2/2}\frac{\cos k\|\mathbf{R}\|}{\|\mathbf{R}\|}\eta_{x,y}(x',y')\phi(x',y')g(x',y')dx'dy' \\
I(x,y) &= \int_{x-d_1/2}^{x+d_1/2}\int_{y-d_2/2}^{y+d_2/2}\left(\frac{\cos k\|\mathbf{R}\|}{\|\mathbf{R}\|}+k\sin k\|\mathbf{R}\|\right)\frac{\mathbf{R}\cdot(-f_{x'},-f_{y'},1)}{4\pi\|\mathbf{R}\|^2}e^{i\alpha(x'-x)}e^{i\beta(y'-y)} \\
&\times \eta_{x,y}(x',y')\phi(x',y')dx'dy'
\end{aligned}$$

where $\mathbf{R} = (x - x', y - y', f(x,y) - f(x',y'))$ is based on *analytic resolution* of singularities via changes of variables to polar coordinates [5]. These require introducing a system of polar coordinates centered at $(x,y):\ x' = x + \rho\cos\theta,\ y' = y + \rho\sin\theta$. Accordingly, the singular integrals are cast into the form

$$I(x,y) = \int_0^\pi L_{SL}(x,y,\theta)d\theta, \quad J(x,y) = \int_0^\pi L_{DL}(x,y,\theta)d\theta \tag{54}$$

where

$$\begin{aligned} L_{SL}(x,y,\theta) &= \int_{-r_1}^{r_1} f^*_{SL}(\rho,\theta)\frac{|\rho|}{\|\mathbf{R}\|}\cos k\|\mathbf{R}\|d\rho \\ L_{DL}(x,y,\theta) &= \int_{-r_1}^{r_1} f^*_{DL}(\rho,\theta)\left(\frac{|\rho|}{\|\mathbf{R}\|}\right)^3(\cos k\|\mathbf{R}\| + k\|\mathbf{R}\|\sin k\|\mathbf{R}\|)\frac{\mathbf{R}\cdot(-f_{x'},-f_{y'},1)}{4\pi|\rho|^2}d\rho \end{aligned} \tag{55}$$

with

$$\mathbf{R} = \mathbf{R}(\rho,\theta) = (-\rho\cos\theta, -\rho\sin\theta, f(x,y) - f(x+\rho\cos\theta, y+\rho\sin\theta))$$

and

$$f^*_{SL} = \phi(x+\rho\cos\theta, y+\rho\sin\theta)\eta_{x,y}(x+\rho\cos\theta, y+\rho\sin\theta)g(x+\rho\cos\theta, y+\rho\sin\theta)e^{i\alpha\rho\cos\theta}e^{i\beta\rho\sin\theta}$$

$$f^*_{DL} = \phi(x+\rho\cos\theta, y+\rho\sin\theta)\eta_{x,y}(x+\rho\cos\theta, y+\rho\sin\theta)e^{i\alpha\rho\cos\theta}e^{i\beta\rho\sin\theta}.$$

For a smooth surface, the expressions $\frac{|\rho|}{\|\mathbf{R}\|}$ are smooth functions of ρ for any fixed direction of θ. In the limit $\rho \to 0$, the value of $\frac{|\rho|}{\|\mathbf{R}\|}$ is

$$\lim_{\rho\to 0}\frac{|\rho|}{\|\mathbf{R}\|} = \frac{1}{(1 + (f_x\cos\theta + f_y\sin\theta)^2)^{1/2}}. \tag{56}$$

The expressions $\frac{\mathbf{R}\cdot(-f_{x'},-f_{y'},1)}{|\rho|^2}$ are also smooth functions of ρ for any fixed direction of θ. In the limit $\rho \to 0$, the value of $\frac{|\rho|}{\|\mathbf{R}\|}$ is

$$\lim_{\rho\to 0}\frac{\mathbf{R}\cdot(-f_{x'},-f_{y'},1)}{|\rho|^2} = \frac{1}{2}(f_{xx}\cos^2\theta + 2f_{xy}\cos\theta\sin\theta + f_{yy}\sin^2\theta). \tag{57}$$

As all the factors in the integrands in the radial integration are smooth and vanish with their derivatives at the endpoints of integration, the trapezoidal rule yields high-order accuracy results; subsequently, the angular integration assumes integrands that are smooth and periodic functions of θ, and, thus, an extra application of the trapezoidal rule will produce an overall high-order integration method for the singular adjacent interactions. More precisely, we consider an equi-spaced grid in θ such that $\theta_\ell = \ell\Delta\theta,\ \ell = 0,\dots n_\theta - 1$, where $\Delta\theta = \frac{\pi}{n_\theta}$ and an equi-spaced grid in ρ such that $\rho_j = -r_1 + j\Delta\rho,\ j = 1,\dots n_\rho - 1$ where $\Delta\rho = \frac{2r_1}{n_\rho}$. An application of the trapezoidal rule gives

$$I(x_p,y_q) \approx \Delta\rho\ \Delta\theta\sum_{l=0}^{n_\theta-1}\sum_{j=1}^{n_\rho-1} f^*_{SL}(\rho_j,\theta_\ell)\frac{|\rho_j|}{\|\mathbf{R}(\rho_j,\theta_\ell)\|}\cos k\|\mathbf{R}(\rho_j,\theta_\ell)\|.$$

and

$$\begin{aligned} J(x_p,y_q) &\approx \Delta\rho\ \Delta\theta\sum_{l=0}^{n_\theta-1}\sum_{j=1}^{n_\rho-1} f^*_{DL}(\rho_j,\theta_\ell)\left(\frac{|\rho_j|}{\|\mathbf{R}(\rho_j,\theta_\ell)\|}\right)^3\frac{\mathbf{R}(\rho_j,\theta_\ell)\cdot(-f_{x'},-f_{y'},1)}{|\rho_j|^2} \\ &\times (\cos k\|\mathbf{R}(\rho_j,\theta_\ell)\| + k\|\mathbf{R}(\rho_j,\theta_\ell)\|\sin k\|\mathbf{R}(\rho_j,\theta_\ell)\|). \end{aligned}$$

The fact that the radial quadrature points resulted from the analytic resolution of the singularity $(x_p + \rho_j \cos\theta_\ell, y_q + \rho_j \sin\theta_\ell)$ do not lie on the Cartesian grid associated with the given coordinate patch can be dealt efficiently through 2D discrete Fourier transforms that are effected efficiently via FFTs. Indeed, assuming that N is even we have that

$$\phi(x,y) \approx \sum_{j=-N/2+1}^{N/2} \sum_{\ell=-N/2+1}^{N/2} \hat{\phi}_{j\ell} e^{\frac{2\pi i j x}{d_1}} e^{\frac{2\pi i \ell y}{d_2}}$$

where $\hat{\phi}_{j\ell},\ j,\ell = -N/2+1, \ldots N/2$ denote the discrete Fourier transform of the values $\phi_{pq},\ p,q = 0,\ldots N-1$. We use these discrete Fourier coefficients to evaluate $\phi(x_p + \rho_j \cos\theta_\ell, y_q + \rho_j \sin\theta_\ell)$ for all $p,q = 0,\ldots N-1$ and all $\ell = 0,\ldots n_\theta - 1$ and $j = 1,\ldots,n_\rho$.

6 Numerical results

We present numerical computations of scattering by doubly periodic arrays of obstables and by doubly periodic reflecting gratings. For periodic arrays of obstacles, we compute scattering for non-Wood parameters using a smooth cutoff of the lattice sum for the quasi-periodic Green function. For periodic gratings, we compute scattering at and around Wood parameters using the modified Green function $\tilde{G}_k^{qper,p}$ with a smooth cutoff. In both cases, the computations are accurate and efficient.

We take the incident field to be the $(0,0)$ harmonic incident from the top of the scatterer. In the case of an array of scatterers, the scattered field $u^\pm(\mathbf{x})$ satisfies the outgoing condition given by (7). Conservation of energy serves as a test of numerical accuracy. In the case of a periodic array of scatters, it requires that the energy flux of the incident field equal the energy flux of the reflected field plus the energy flux of the transmitted field. Energy conservation is expressed in terms of the Rayleigh coefficients of the scattering problem,

$$\sum_{(j,\ell)\in P} \gamma_{j\ell} |B_{j\ell}^+|^2 + \sum_{(j,\ell)\in P} \gamma_{j\ell} |B_{j\ell}^- + \delta_{j\ell}^{00}|^2 = \gamma_{00}\,, \tag{58}$$

where P is the set of propagating harmonics $P = \{(j,\ell) : \alpha_j^2 + \beta_\ell^2 \le k^2\} = \{(j,\ell) : \gamma_{j\ell} > 0\}$.

To assess the accuracy of the computations, we compute (1) the energy error defined as

$$\epsilon = \frac{\left|\sum_{(j,\ell)\in P} \gamma_{j\ell}\big(|B_{j\ell}^+|^2 + |B_{j\ell}^- + \delta_{j\ell}^{00}|^2\big) - \gamma_{00}\right|}{\gamma_{00}}$$

and (2) precision error in the Rayleigh coefficient $B_{0,0}^-$ which we denote by ϵ_1. The latter errors are computed using as reference solutions those obtained by choosing large values of the parameter a in the definition of $G_k^{a,per}$ and refined discretizations. The solution of the linear systems resulting from our discretization was obtained using a GMRES solver with a relative residual tolerance of 10^{-4}.

We present computations of scattering for periodic arrangements of spheres and cubes, both of which have diameter equal to 2. The periods are $d_1 = d_2 = 4$, and plane wave normal incidence, that is $\psi = \phi = 0$, or equivalently $\alpha = \beta = 0$. Table 1 shows results for periodic arrays of spheres and cubes for various wavenumbers k as we increase the values of the parameter a in the definition of $G_k^{a,per}$. Specifically, we present the errors ϵ and ϵ_1 defined above together with the number of iterations and the total computational times required by the GMRES solvers to reach a relative

Scatterer	k	Unknowns	a	ϵ	ϵ_1	Iter	Time
Sphere	0.75	$6 \times 16 \times 16$	20	6.5×10^{-3}	6.2×10^{-3}	6	18sec
Sphere	0.75	$6 \times 16 \times 16$	30	3.5×10^{-4}	2.1×10^{-3}	6	33sec
Sphere	0.75	$6 \times 16 \times 16$	40	1.9×10^{-5}	3.3×10^{-4}	6	55sec
Sphere	8	$6 \times 32 \times 32$	20	7.8×10^{-3}	6.2×10^{-3}	20	1m45sec
Sphere	8	$6 \times 32 \times 32$	30	3.0×10^{-3}	2.1×10^{-3}	20	2m22sec
Sphere	8	$6 \times 32 \times 32$	60	6.0×10^{-4}	3.3×10^{-4}	20	5m21sec
Cube	0.75	$6 \times 16 \times 16$	20	2.2×10^{-3}	0.1×10^{-2}	12	26sec
Cube	0.75	$6 \times 16 \times 16$	30	1.1×10^{-4}	6.2×10^{-3}	11	40sec
Cube	0.75	$6 \times 16 \times 16$	40	3.0×10^{-5}	1.4×10^{-3}	11	1m2sec

Table 1: Convergence of the periodic solvers using $G_k^{a,per}$ for increasing values of the windowing parameter a for doubly periodic arrays of spheres and cubes.

residual of 10^{-4}. The results were obtained by a C++ implementation of our solvers on a machine with 2.67 GHz Intel Xeon CPUs and 24Gb of RAM.

With regard to computational times, the implementation of one of the most advanced techniques for evaluation of periodic Green functions [11], which is based on Kummer transforms, either spatial or spectral representations, supplemented by Shanks transforms, is reported to take several miliseconds [2]. Thus, for a discretization $6 \times 16 \times 16$ there are about 1.8×10^6 evaluations of periodic Green functions which will require at least 1.8×10^3 seconds to evaluate one matrix vector product. In contrast, as it can be seen in Table 1, in the case of periodic two-dimensional arrays of spheres, our solvers require about 55 sec to obtain results with four digits of accuracy.

For scattering off of doubly periodic gratings, we take the periods to be $d_1 = d_2 = 1$. The energy conservation law states that the energy of the incident wave equals the energy of the reflected wave,

$$\sum_{(j,\ell)\in P} \gamma_{j\ell} |B^+_{j\ell}|^2 = \gamma_{00}. \tag{59}$$

We compute the following performance metric associated with the conservation of energy,

$$\epsilon = \frac{\left|\sum_{(j,\ell)\in P} \gamma_{j\ell} |B_{j\ell}|^2 - \gamma_{00}\right|}{\gamma_{00}}. \tag{60}$$

In addition to measures of conservation of energy, we present numerical errors incurred in the coefficient $B^a_{0,0}$ resulting from the use of $G_k^{a,per}$ for various values of the truncation parameter a with respect to a reference coefficient $B^A_{0,0}$ obtained through refined discretizations and large enough values of the parameter A so that the quasi-periodic Green function $G_k^{A,per}$ has many digits of accuracy (typically at least 10). We denote these errors by ϵ_1. We note that for large enough values of the truncation parameter A, the accuracy of the solver is limited by the accuracy of the singular integrator. All linear systems resulting form the high-order discretization of the periodic boundary-integral equations for solutions of scattering problems off gratings were solved using GMRES with a relative tolerance of 10^{-6}.

We consider in Tables 2-5 the doubly periodic grating $f(x,y) = \frac{1}{2}\cos(2\pi x)\cos(2\pi y)$ and various values of the wavenumber k, away from as well as at and around Wood frequencies. We present in Table 2 the high-order nature of our solvers with Dirichlet boundary conditions using the windowing

k	Unknowns	a	$\max \lvert G^a - G^A \rvert$	Iter	ϵ_1	ϵ
1	8×8	30	4.4×10^{-2}	10	2.0×10^{-2}	4.0×10^{-2}
1	8×8	60	3.1×10^{-3}	10	1.8×10^{-3}	2.0×10^{-3}
1	16×16	120	2.3×10^{-4}	10	5.4×10^{-4}	7.1×10^{-4}
1	16×16	160	3.7×10^{-5}	10	1.3×10^{-4}	2.3×10^{-4}

Table 2: Convergence of the solvers using G^a, away from Wood frequencies, normal incidence; reference solution corresponds to $A = 240$, 16×16 unkowns, for which $\epsilon = 1.1 \times 10^{-5}$.

k	Unknowns	a	G^a			$G^{a,p}, p = 3$		
			Iter	ϵ_1	ϵ	Iter	ϵ_1	ϵ
6	16×16	30	16	4.9×10^{-3}	1.6×10^{-3}	12	6.5×10^{-3}	1.2×10^{-2}
6	16×16	60	16	1.5×10^{-3}	4.1×10^{-4}	12	3.8×10^{-4}	1.5×10^{-5}

Table 3: Convergence of the solvers using G^a and $G^{a,p}, p = 3, d = 2.4$, away from Wood frequencies, normal incidence; reference solution corresponds to $A = 120$, 32×32 unkowns, for which $\epsilon = 4.0 \times 10^{-7}$.

functions G^a for increasing values of the windowing parameter a and values of k away from Wood anomalies.

We present in Table 3 the high-order nature of our scattering solvers with Dirichlet boundary conditions using the windowing functions G^a and the shifted windowing functions $G^{a,p}, p = 3$ for increasing values of the windowing parameter a and values of k away from Wood anomalies.

We turn next in Table 4 to the case of Wood and near Wood anomalies. In the case of normal incidence the first three Wood anomalies occur at $k = 2\pi$, $k = 2\sqrt{2}\pi$, and $k = 4\pi$. We illustrate in Table 4 the high-order convergence of our solvers based on the shifted windowing Green functions $G^{a,p}$ for a value of the shift given by $d = 1.4$. We note that the number of iterations required by the GMRES solvers based on Combined Field Integral Equations remains small even for Wood and near-Wood parameters.

In Table 5 we perform the same scattering experiments as in Table 4 but for Neumann boundary conditions. Finally, we illustrate in Figure 3 the behavior of the amplitudes of the Rayleigh modes $B_{0,0}$, $B_{-1,-1}$, and $B_{-1,1}$ as a function of the incidence angle ψ in the neighborhood of the value $\psi_0 = \pi/4$ for wavenumber $k = 2\sqrt{2}\pi$. The case $k = 2\sqrt{2}\pi$ and $\psi_0 = \pi/4$, $\phi = 0$ is a Wood anomaly since $\gamma_{0,1} = 0$.

k	Unknowns	a	Iter	ϵ_1	ϵ
2π	24×24	20	19	3.2×10^{-2}	1.7×10^{-2}
2π	24×24	30	19	2.7×10^{-3}	4.7×10^{-3}
2π	24×24	40	19	6.9×10^{-4}	4.0×10^{-4}
$2\pi \pm 10^{-6}$	24×24	40	19	6.8×10^{-4}	4.3×10^{-4}
$2\sqrt{2}\pi$	24×24	30	25	1.3×10^{-2}	1.5×10^{-2}
$2\sqrt{2}\pi$	24×24	40	25	6.8×10^{-3}	5.5×10^{-3}
$2\sqrt{2}\pi \pm 10^{-6}$	24×24	30	25	1.6×10^{-2}	2.5×10^{-3}
$2\sqrt{2}\pi \pm 10^{-6}$	24×24	40	25	3.4×10^{-3}	6.2×10^{-3}
4π	32×32	30	28	4.6×10^{-2}	4.9×10^{-2}
4π	32×32	40	28	7.4×10^{-3}	6.5×10^{-3}

Table 4: Convergence of the Dirichlet solvers at and around Wood frequencies using $G^{a,p}$, $p = 3$, shift $d = 1.4$ GMRES residual equal to 10^{-6}. The reference solutions correspond to (i) $a = 60$ for $k = 2\pi$, in which case the conservation of energy error is equal to $\epsilon = 2.4 \times 10^{-6}$; (ii) $a = 60$ for $k = 2\sqrt{2}\pi$, in which case the conservation of energy error is equal to $\epsilon = 6.3 \times 10^{-4}$; (iii) $a = 60$ for $k = 4\pi$, in which case the conservation of energy error is equal to $\epsilon = 2.0 \times 10^{-3}$.

k	Unknowns	a	Iter	ϵ_1	ϵ
2π	24×24	20	19	5.3×10^{-3}	7.4×10^{-3}
2π	24×24	30	19	5.7×10^{-4}	1.7×10^{-3}
2π	24×24	40	19	1.1×10^{-4}	3.7×10^{-4}
$2\pi \pm 10^{-6}$	24×24	40	19	1.1×10^{-4}	3.6×10^{-4}
$2\sqrt{2}\pi$	24×24	30	25	5.3×10^{-2}	1.0×10^{-1}
$2\sqrt{2}\pi$	24×24	50	25	1.7×10^{-2}	3.3×10^{-2}
$2\sqrt{2}\pi \pm 10^{-6}$	24×24	50	25	1.2×10^{-2}	2.2×10^{-2}
4π	32×32	30	28	1.2×10^{-1}	4.5×10^{-2}
4π	32×32	60	28	1.4×10^{-2}	1.6×10^{-2}
$2\pi \pm 10^{-6}$	32×32	60	28	1.4×10^{-2}	1.6×10^{-2}

Table 5: Convergence of the Neumann solvers at and around Wood frequencies using $G^{a,p}$, $p = 3$, shift $d = 1.4$ GMRES residual equal to 10^{-6}. The reference solutions correspond to (i) $a = 60$ for $k = 2\pi$, in which case the conservation of energy error is equal to $\epsilon = 2.4 \times 10^{-6}$; (ii) $a = 80$ for $k = 2\sqrt{2}\pi$, in which case the conservation of energy error is equal to $\epsilon = 2.8 \times 10^{-3}$; (iii) $a = 80$ for $k = 4\pi$, in which case the conservation of energy error is equal to $\epsilon = 1.1 \times 10^{-3}$.

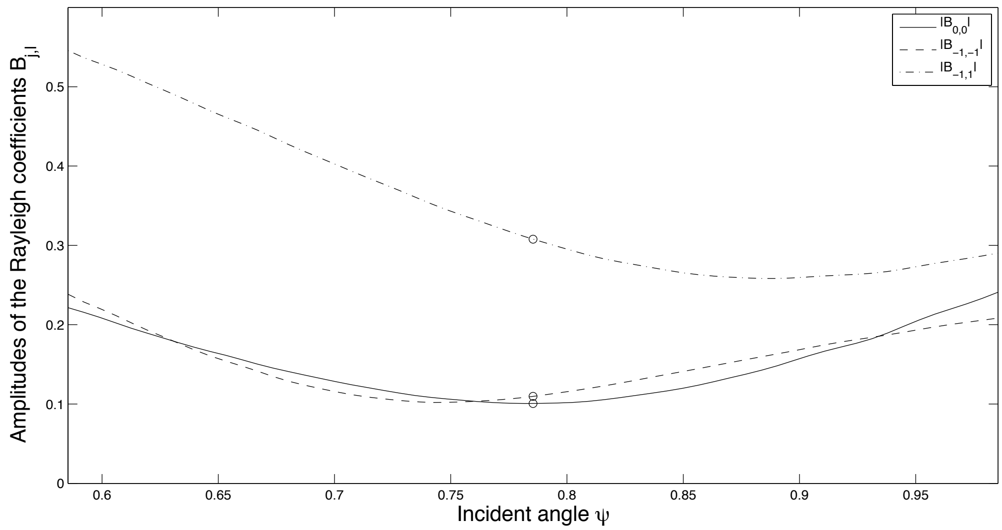

Figure 3: Plot of the amplitudes of the Rayleigh modes $|B_{0,0}|$, $|B_{-1,-1}|$, and $|B_{-1,1}|$ for the wavenumber $k = 2\sqrt{2}\pi$ as a function of the azymuthal angle ψ around the value $\psi_0 = \pi/4$. We took $\phi = 0$ in all of these experiments. For incidence angles $\psi_0 = \pi/4$ and $\phi = 0$, the value $k = 2\sqrt{2}\pi$is a Wood anomaly since $\gamma_{0,1} = 0$. We considered 60 values of the incidence angle ψ in a small neighborhood of $\psi_0 = \pi/4$. The values of the Rayleigh amplitudes at the Wood frequency corresponding to $\psi_0 = \pi/4$ are depicted by $\circ$. For each scattering experiment we computed the conservation of energy error ϵ and the magnitude of those did not exceed 2%.

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