An integral representation of the Green function for a linear array of acoustic point sources

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Abstract

We present a new algorithm for the evaluation of the quasi-periodic Green function for a linear array of acoustic point sources such as those arising in the analysis of line array loudspeakers. A variety of classical algorithms (based on spatial and spectral representations, Ewald transformation, etc.) have been implemented in the past to evaluate these acoustic fields. However as we show, these methods become unstable and/or impractically expensive as the frequency of use of the sources increases. Here we introduce a new numerical scheme that overcomes some of these limitations allowing for simulations at unprecedentedly large frequencies. The method is based on a new integral representation derived from the classic spatial form, and on suitable further manipulations of the relevant integrands to render the integrals amenable to efficient and accurate approximations through standard quadrature formulas. We include a variety of numerical results that demonstrate that our algorithm compares favorably with several classical methods both for points close to the line where the poles are located and at high-frequencies while remaining competitive with them in every other instance.

Key words: Green function, periodic domain, rough-surface, high-frequency, free-space, Helmholtz equation.

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1 Introduction

The evaluation of the potential due to an infinite number of acoustic point sources arranged periodically along a line in three space dimensions presents numerical challenges. Knowledge of this potential is useful, for example, in the design of line array loudspeakers. These are collections of speakers arranged in a vertical or horizontal configuration; patterns of constructive and destructive interference lead to more directionality and sound intensity compared to a single speaker. The effects of increased directionality were documented in [1]. Another interesting feature of these speakers is that in certain limits, the intensity of acoustic power varies inversely with the distance, rather than inversely with the square of the distance as one might expect with a radiating point source. Since the 1960s, such line array speakers have become popular especially in large venues. Challenges arise with faithful sound reproduction in the near field as well as in the high-frequency domain, and the ability to rapidly and accurately compute the potential due to such an arrangement of sources is key in the optimal design of such speakers. In this paper we introduce a novel method for the evaluation of this potential (the Green function). The method is applicable even in the regimes where existing methods are not competitive.

The general area of computing quasi-periodic Green functions has attracted significant attention from engineers and mathematicians over the last 40 years and has resulted in some novel methods, including the work in [2–5] for two-dimensional problems with one-dimensional periodicity (i.e., a planar array of line sources) and [6,7] for three-dimensional problems with two-dimensional periodicity (i.e., a planar array of point sources). Indeed, while the present paper describes an intermediate problem of one-dimensional periodicity in three dimensions [8–10], part of the motivation is to use this method as a building block for the full three-dimensional problem with two-dimensional periodicity. A recent work by Linton [11] provides an excellent overview of these problems.

The classical algorithms based on using spatial or spectral representations may necessitate an inordinate amount of terms to be included for accurate evaluations (especially at high-frequencies), while the Ewald transform [8–10] results in unavoidable loss of accuracy in certain regimes. We shall show that these algorithms develop problems especially in the extremely near-field, as well as at high-frequencies.

The method we introduce can effectively provide solutions at very high-frequencies or in the very near field, while remaining competitive with the optimal choices of currently available schemes throughout their domain of applicability. Briefly, the method begins with a new integral representation similar to one developed in [5] for the case of a planar array of line sources. The method is based on the

spatial representation of the Green function, G, from which an integral representation is derived. The integrand in the latter is an exponentially decaying function $f(x, y, z; u)$ for $u \geq 0$ where (x, y, z) denote the spatial variables and the sources are placed along the $z-$axis. At low-frequencies and/or for small values of the distance $\rho = \sqrt{x^2 + y^2}$ the function f and its derivatives remain bounded and a standard quadrature can provide an efficient means to evaluate the integral. As the frequency increases, the integrand f displays progressively larger and more rapid oscillations which cancel out to produce a significantly smaller integrated value. In this case classical quadratures tend to be unstable and inadequate. To overcome these difficulties our scheme is based on polynomial expansions of quotients of f and suitably chosen functions to allow for explicit evaluations, and on judicious integration by parts in order to improve stability and reduce the computational cost.

The rest of the paper is organized as follows. First, and for the sake of completeness, in §2 we briefly review the most popular methods that have been devised to compute G, including those based on spatial and spectral representations, and on the Ewald transform. We discuss the problems that arise with each of these, either as the observation point approaches the array or as the frequency increases. In section §3 we derive a new integral representation, §4 is devoted to the presentation of our new high-frequency algorithm and in §5 formulas for the partial derivatives of G are presented. Finally in §6 we present numerical results that confirm that this method significantly outperforms classical procedures. As we show, the method enables accurate simulations even in the regimes where other methods fail.

2 Problem statement and review of existing algorithms

In this paper, we are concerned with the problem of evaluating the scalar potential due to point sources arrayed along a line with equal spacing. These sources are assumed to be operating with equal amplitude and with phases that are allowed to vary linearly with the source location. In [1], the characteristic features of such line arrays are described. For example, the directional behavior of such an array is observed only within a range of frequencies. In order to maintain directionality at high frequencies, it is known that the spacing between the sources must be reduced.

We will be working in the frequency domain, and thus a time dependence of $e^{-i\omega t}$ has been factored out. The point sources are assumed to be located at positions $nd\hat{k}$ for $n \in \mathbb{Z}$, $d > 0$. There is thus a natural periodicity with period d in the z direction. We assume further that the line array is embedded in a medium with background wave number $k \in \mathbb{R}$, and we are interested in the outgoing solution of the Helmholtz equation.

The problem can be rephrased in terms of the (outgoing) Green function $G(x, y, z)$: Find the solution of

$$\Delta G(x, y, z) + k^2 G(x, y, z) = -\sum_{n=-\infty}^{\infty} \delta(x)\delta(y)\delta(z - nd)e^{i\alpha nd},$$

where the nth point source is located at $R_n = nd\hat{k}$ and $\alpha \in \mathbb{R}$.

We shall now describe some popular representations of $G(\rho, z)$ which are used in some existing numerical strategies. We discuss the difficulties which arise in the high-frequency (large k) and nearly-axial (small ρ) regimes. In each case, these difficulties lead to an increase in computational cost and/or the deterioration of the stability properties of these methods.

1. <u>Spatial representation:</u> The simplest method for evaluating $G(\rho, z)$ follows from the explicit knowledge of the free-space Green function G_s with a single point source located at the origin: $G_s(x, y, z) = G_s(\rho, z) = \dfrac{e^{ik\sqrt{\rho^2+z^2}}}{4\pi\sqrt{\rho^2 + z^2}}$. For an array of such point sources, we can simply add these contributions. For fixed α and wave number k :

$$G(\rho, z) = \frac{1}{4\pi} \sum_{n=-\infty}^{\infty} e^{i\alpha nd} \frac{e^{ikr_n}}{r_n} \tag{1}$$

where

$$r_n = \sqrt{\rho^2 + (z - nd)^2}.$$

The terms of this series only decay as $\dfrac{1}{n}$, and the series does not converge absolutely. Therefore, summation of this series is an inefficient technique at best; the problems are independent of frequency. More precisely, for N large:

$$\left| G(\rho, z) - \frac{1}{4\pi} \sum_{n=-N}^{N} e^{i\alpha nd} \frac{e^{ikr_n}}{r_n} \right| \approx \left| \frac{1}{2\pi} \frac{e^{i(N+1)(k+\alpha)d}}{(N + 1)d} \right| = \frac{1}{2\pi(N + 1)d} \tag{2}$$

and for r_0 small:

$$G(\rho, z) \approx \frac{1}{4\pi} \frac{e^{ikr_0}}{r_0}.$$

2. <u>Spectral representation:</u> Another approach for computing G relies on its Fourier series representation [10]. Since G is a (quasi) periodic function, one can easily use Poisson's summation formula to obtain a "spectral representation":

$$\sum_{n=-\infty}^{\infty} f(nd) = \frac{1}{d} \sum_{q=-\infty}^{\infty} \tilde{f}(\frac{2\pi}{d}q),$$

where

$$f(nd) = e^{i\alpha nd}\frac{e^{ikr_n}}{4\pi r_n}, \qquad r_n = \sqrt{\rho^2 + (z - nd)^2},$$

and

$$\tilde{f}(\frac{2\pi}{d}q) = \int_{-\infty}^{\infty} e^{i\frac{2\pi}{d}qu} f(u)du.$$

Indeed letting:

$$\alpha_n = \alpha + \frac{2\pi}{d}n \text{ and } \beta_n = \sqrt{k^2 - \alpha_n^2} \tag{3}$$

this spectral representation becomes:

$$G(\rho, z) = -\frac{1}{4id}\sum_{n=-\infty}^{\infty} e^{i\alpha_n z} H_0^{(1)}(\beta_n \rho), \tag{4}$$

where $H_0^{(1)}$ is the zeroth order Hankel function of the first kind:

$$H_0^{(1)}(z) = J_0(z) + iY_0(z)$$

and $J_0(z)$, $Y_0(z)$ are the zeroth order Bessel functions of the first and second kind respectively.

In contrast with the representation in (1) the series in (4) converges exponentially for $\rho > 0$. If α is real and the medium is lossless (k is real), then for $\alpha_n^2 < k^2$ the β_n describe radially propagating waves, while for $\alpha_n^2 > k^2$ the β_n index waves attenuating in the ρ direction. The critical index is

$$N = \frac{|k|d - \alpha d}{2\pi};$$

for $|n| > N$ the terms in the series (4) decay exponentially, corresponding to the attenuating modes. This is easily seen from the asymptotic behavior of the Hankel function:

$$H_0^{(1)}(a) \sim \sqrt{\frac{2}{\pi a}} e^{i(a - \frac{\pi}{4})} \quad \text{for } 1 \ll |a| \text{ [12, Eq. 9.2.3].}$$

Clearly if β_n is complex-valued, which happens for $|n| > N$, $H_0^{(1)}(\beta_n\rho)$ is an exponentially small term *provided* $\rho > 0$. The method does not converge if $\rho = 0$.

It is worth examining the computational cost of this method. We would need to retain, at a minimum, enough terms n in the series such that $|\beta_n|\rho > 1$. For example, $n > N$ must be chosen large enough such that $|\beta_n|\rho = \left|\sqrt{k^2 - (\alpha + \frac{2\pi}{d}n)^2}\right|\rho > 1$ or, equivalently

$$n > 2N + \frac{2}{\rho\frac{2\pi}{d}\left(k\rho + \sqrt{k\rho^2 + 1}\right)}. \tag{5}$$

Clearly if k is large, or ρ/d is small, n must be chosen to be large enough to provide accurate results.

3. <u>Ewald transformation:</u> The Ewald summation technique for this problem [8–10] is based on the integral representation:

$$\frac{e^{ikr}}{4\pi r} = \frac{1}{2\pi^{3/2}} \int_0^\infty e^{-r^2 s^2 + \frac{k^2}{4s^2}} ds,$$

to accelerate the convergence of the spatial representation series in (1). To review this approach, let us begin with fixing $E > 0$, and defining:

$$G_{\text{spectral}}(\rho, z) = \frac{1}{2\pi\sqrt{\pi}} \sum_{n=-\infty}^{\infty} e^{i\alpha nd} \int_0^E e^{-r_n^2 s^2 + \frac{k^2}{4s^2}} ds,$$

and

$$G_{\text{spatial}}(\rho, z) = \frac{1}{2\pi\sqrt{\pi}} \sum_{n=-\infty}^{\infty} e^{i\alpha nd} \int_E^\infty e^{-r_n^2 s^2 + \frac{k^2}{4s^2}} ds,$$

where $r_n = \sqrt{\rho^2 + (z - nd)^2}$ so that, from (1),

$$G(\rho, z) = G_{\text{spectral}}(\rho, z) + G_{\text{spatial}}(\rho, z). \tag{6}$$

Next we note that the series $G_{\text{spectral}}(\rho, z)$ rewritten as:

$$G_{\text{spatial}}(\rho, z) = \frac{1}{8\pi} \sum_{n=-\infty}^{\infty} \frac{e^{i\alpha nd}}{r_n} \left[e^{-ikr_n} \text{erfc}(Er_n - i\frac{k}{2E}) + e^{ikr_n} \text{erfc}(Er_n + i\frac{k}{2E}) \right], \tag{7}$$

where $\text{erfc}(a)$ is the complementary error function. The other series G_{spectral}, in turn, can be written as:

$$G_{\text{spectral}}(\rho, z) = \frac{1}{4\pi d} \sum_{n=-\infty}^{\infty} e^{i\alpha_n z} \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} (\rho E)^{2m} E_{m+1}(-\frac{\beta_n^2}{4E^2}), \tag{8}$$

where the mth order exponential integral $E_m(x)$ is defined by

$$E_m(x) = \int_1^\infty u^{-m} e^{-xu} du$$

and β_n defined in (3). Now, the combined exponential decay of the series (7) and (8) make this into an efficient method for moderate values of k. In this case, it can be shown that the optimal choice of E is

$$E \approx \frac{\sqrt{\pi}}{d}, \tag{9}$$

in which case both series converge at the same asymptotic rate [10]. However, as also shown in [10,13], this choice of the parameter E leads to unstable evaluations for larger frequencies and must be modified to ensure the boundedness

of the terms in the series. More precisely, we have:

$$\mathrm{erfc}(a) \sim e^{-a^2}/\sqrt{\pi a} \text{ and } E_1(a) \sim e^{-a}/a \text{ for } |a| \gg 1,$$

so that, for large k:

$$G_{\text{spatial}}(\rho, z) \sim \sum_n e^{\frac{k^2}{4E^2} - E^2(\rho^2 + (z-nd)^2)},$$

and

$$G_{\text{spectral}}(\rho, z) \sim \sum_n \frac{4E^2}{k^2 - (\alpha + np)^2} e^{\frac{k^2 - (\alpha+np)^2}{4E^2}}.$$

Thus, for large k, a choice of E that is independent of frequency (such as that in (9) leads to large values of the terms in the series (7) and (8) and to inaccurate values of the $G(\rho, z)$ as a result of cancelations. To avoid this difficulty, one may choose:

$$E = \max\left\{E_{\text{spectral}} = \frac{C_1\sqrt{k}}{\sqrt{2\sqrt{\rho^2 + z^2}}},\ E_{\text{spatial}} = \frac{C_2\sqrt{k^2 - \alpha^2}}{2}\right\} \tag{10}$$

for some constants $C_{1,2}$ which are related to the maximum allowable value of the terms in (7) and (8).

As can be easily verified this choice will allow evaluations of $G_{\text{spatial}}(\rho, z)$ with a computational cost independent of frequency and will put the computational burden on the calculation of $G_{\text{spectral}}(\rho, z)$. In detail, we can approximate:

$$G_{\text{spectral}} \approx \frac{1}{4\pi d} \sum_{n=-N}^{N} e^{i\alpha_n z} \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} (\rho E)^{2m} E_{m+1}(-\frac{\beta_n^2}{4E^2}) \tag{11}$$

to within an accuracy of ϵ provided:

$$N \geq \log(\epsilon) k,$$

and this, in turn, leads to a computational cost that is similar to that of evaluation of standard spectral series (4).

Moreover, once E chosen as in (10), its stability properties deteriorate significantly for large k due to the correspondingly large values of

$$\frac{(\rho E)^{2m}}{m!} \sim \max\left\{\frac{\left(k\rho^2/\sqrt{\rho^2 + z^2}\right)^m}{m!}, \frac{(k\rho)^{2m}}{m!}\right\} \tag{12}$$

in the inner sum (11), (see also [10, §4.2]) resulting an unavoidable loss of accuracy in its evaluation.

3 A new integral representation of the Green function

In this section we will derive an alternative representation for the Green function for a line array. This representation will form the backbone of our computational method. As in [5,9], the starting point for this derivation is the spatial form (1), and the simple observation that:

$$\sum_{n=1}^{\infty} e^{-ian} e^{-nv} = \frac{e^{-ia}}{e^{v} - e^{-ia}}.$$

If $F = L(f)$ is the Laplace transform of a function f, then we can use the identity above to get:

$$\sum_{n=1}^{\infty} e^{-ian} F(n) = e^{-ia} \int_0^{\infty} \frac{f(v)}{e^{v} - e^{-ia}} dv.$$

For our purposes, we use the identity [14, Eq. 4.15.19] for $|\arg \beta| < \pi$:

$$L^{-1}\{e^{\beta m} \frac{e^{-\beta\sqrt{m^2+\gamma^2}}}{\sqrt{m^2+\gamma^2}}\} = J_0(\gamma\sqrt{v^2 + 2\beta v}) \text{ for } \Re(m) > |\Im(\beta)|$$

to see that for $n > 0$, the sum in (1) becomes:

$$\sum_{n=1}^{\infty} e^{i\alpha nd} \frac{e^{ikr_n}}{r_n} = \int_0^{\infty} \frac{e^{ikd}}{e^{v} - e^{ikd}} \left(\frac{1}{d} e^{-ikz + \frac{z}{d}v} J_0\Big(\rho\sqrt{(\frac{v}{d})^2 - 2ik\frac{v}{d}}\Big) \right) dv.$$

We can use a similar argument for the remaining terms of the sum in (1):

$$\begin{aligned}\sum_{n=-\infty}^{-1} e^{i\alpha nd} \frac{e^{ikr_n}}{r_n} &= \sum_{n=1}^{\infty} e^{-i\alpha nd} \frac{e^{ik\sqrt{(z+nd)^2+\rho^2}}}{\sqrt{(z+nd)^2+\rho^2}} \\ &= \int_0^{\infty} \frac{e^{i(k-\alpha)d}}{e^{v} - e^{i(k-\alpha)d}} \left(\frac{1}{d} e^{ikz - \frac{z}{d}v} J_0\Big(\rho\sqrt{(\frac{v}{d})^2 - 2ik\frac{v}{d}}\Big) \right) dv\end{aligned}$$

Putting these expressions together, the Green function $G(\rho, z)$ can be written as:

$$\begin{aligned}G(\rho, z) = \frac{1}{4\pi}\frac{e^{ikr_0}}{r_0} &+ \frac{e^{ikz}}{4\pi d} \int_0^{\infty} \frac{e^{i(k-\alpha)d}}{e^{v} - e^{i(k-\alpha)d}} e^{-\frac{z}{d}v} J_0\Big(\rho\sqrt{(\frac{v}{d})^2 - 2ik\frac{v}{d}}\Big) dv \\ &+ \frac{e^{-ikz}}{4\pi d} \int_0^{\infty} \frac{e^{i(k+\alpha)d}}{e^{v} - e^{i(k+\alpha)d}} e^{\frac{z}{d}v} J_0\Big(\rho\sqrt{(\frac{v}{d})^2 - 2ik\frac{v}{d}}\Big) dv.\end{aligned}$$

Next, a change of variables $v = kd\zeta^2$ (rather than the one $v = kd\zeta$ suggested in [9, Eq. 44]) is applied to put this in a more convenient form:

$$G(\rho, z) = \frac{1}{4\pi}\frac{e^{ikr_0}}{r_0} + \frac{k}{2\pi}\left[\int_0^{\infty} f^{+}(\zeta) d\zeta + \int_0^{\infty} f^{-}(\zeta) d\zeta \right] \tag{13}$$

with

$$f^{\pm}(\zeta) = \zeta \frac{e^{kz(\mp\zeta^2 \pm i)}}{e^{\pm i\alpha d} e^{kd(\zeta^2 - i)} - 1} J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big),$$

which provides the desired representation.

In what follows, and for the sake of the presentation, we shall assume $\alpha = 0$, and focus on the plane $z = 0$. The arguments for other values of α and z follow largely along the same lines (see Appendix A for the general case). In this case, we note that $G(\rho, 0)$ in (13) can be rewritten as:

$$G(\rho, 0) = \frac{1}{4\pi} \frac{e^{ik\rho}}{\rho} + \frac{k}{\pi} \int_0^\infty f(\zeta) d\zeta \tag{14}$$

where

$$f(\zeta) = \zeta \frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big)}{e^{kd(\zeta^2 - i)} - 1}. \tag{15}$$

For a further manipulation of (14), we first expand the denominator of the integrand in (15)

$$\frac{1}{e^{kd(\zeta^2 - i)} - 1} = \frac{1}{e^{(M+1)kd(\zeta^2 - i)} - e^{Mkd(\zeta^2 - i)}} + \sum_{j=1}^{M} \frac{1}{e^{jkd(\zeta^2 - i)}} \tag{16}$$

to rewrite the integral in (14) as:

$$\begin{aligned} \int_0^\infty \zeta \frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big)}{e^{kd(\zeta^2 - i)} - 1} d\zeta = & \int_0^\infty f_{\mathrm{M}}(\zeta) d\zeta \\ & + \sum_{j=1}^{M} e^{ijkd} \int_0^\infty \zeta \frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big)}{e^{jkd\zeta^2}} d\zeta \end{aligned} \tag{17}$$

where

$$f_{\mathrm{M}}(\zeta) = \zeta \frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big)}{e^{(M+1)kd(\zeta^2 - i)} - e^{Mkd(\zeta^2 - i)}}. \tag{18}$$

Finally $G(\rho, 0)$ in (14) can be rewritten:

$$\begin{aligned} G(\rho, 0) = & \frac{1}{4\pi} \frac{e^{ik\rho}}{\rho} + \frac{k}{\pi} \int_0^\infty f_{\mathrm{M}}(\zeta) d\zeta \\ & + \frac{k}{\pi} \sum_{j=1}^{M} e^{ijkd} \int_0^\infty \zeta \frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big)}{e^{jkd\zeta^2}} d\zeta \end{aligned} \tag{19}$$

which provides a new representation of the Green function. As we show in the next section this representation allows further manipulations that can provide the basis for a robust algorithm especially at high-frequencies.

4 A new algorithm

In this section we provide a derivation of a new procedure based on the new integral representation described in the previous section. More precisely, it relies on further manipulation of the integrals in (19) in a manner so as to reduce the integration problem to one where the application of classical quadrature formulas becomes simultaneously stable and efficient.

To begin with we analyze the truncation of the integrals given in (14) and (19) and show that the latter, with a proper choice of M, can be accurately approximated with a smaller integration interval than the former.

Lemma 4.1 *Given $\epsilon > 0$, there exists a $C \in \mathbb{R}$ such that:*

$$|\int_0^\infty f(\zeta)d\zeta - \int_0^C f(\zeta)d\zeta| < \epsilon\frac{\sqrt{\pi}}{\sqrt{4kd}}$$

where C satisfies:

$$\frac{e^{k\rho C}}{e^{kdC^2}} = \epsilon \text{ or, equivalently, } C = \frac{\rho + \sqrt{\rho^2 - \frac{4d\log(\epsilon)}{k}}}{2d}. \tag{20}$$

To see (4.1), we will use:

$$|J_0(a)| \leq e^{|\Im(a)|} \text{ for all } a \text{ [12, Eq. 9.1.62]},$$
$$|\Im(\zeta\sqrt{\zeta^2 - 2i})| = \zeta\sqrt{\frac{2}{\zeta^2 + \sqrt{\zeta^2+4}}} \leq \min\{\zeta, 1\} \text{ for all } \zeta \geq 0,$$

and

$$\zeta e^{k\rho\min\{\zeta,1\}} \leq e^{k\rho\zeta} \text{ for all } \zeta \geq 0.$$

From these it follows:

$$|\zeta\frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{e^{kd(\zeta^2-i)}-1}| \leq |\frac{\zeta e^{k\rho\zeta\sqrt{2/(\zeta^2+\sqrt{\zeta^2+4})}}}{e^{kd(\zeta^2-i)}-1}| \leq |\frac{\zeta e^{k\rho\min\{\zeta,1\}}}{e^{kd(\zeta^2-i)}-1}| \leq |\frac{e^{k\rho\zeta}}{e^{kd(\zeta^2-i)}-1}|.$$

Finally

$$|\int_C^\infty f(\zeta)\,d\zeta| \leq \int_C^\infty |f(\zeta)|\,d\zeta \leq 2\int_C^\infty e^{k\rho\zeta - kd\zeta^2}\,d\zeta \leq \epsilon\frac{\sqrt{\pi}}{\sqrt{4kd}}$$

since

$$|\frac{1}{e^{kd(\zeta^2-i)}-1}| \leq |\frac{2}{e^{kd(\zeta^2-i)}}| \text{ for } u \geq C \text{ if } \epsilon \leq 1,$$

and

$$\int_C^\infty \frac{e^{k\rho\zeta}}{e^{kd\zeta^2}}\,d\zeta = \frac{e^{k\rho C}}{e^{kdC^2}}\int_0^\infty \frac{e^{k\rho v - 2kdCv}}{e^{kdv^2}}\,dv \leq \epsilon\frac{\sqrt{\pi}}{\sqrt{4kd}}$$

provided C is chosen as in (20).

On the other hand, to establish an appropriate truncation for the integral in (19) we begin by noting that for a given ϵ the first integral in (19) can be truncated to $[0, C_{\mathrm{M}}]$ where

$$\frac{e^{k\rho C_{\mathrm{M}}}}{e^{kMdC_{\mathrm{M}}^2}} = \epsilon \text{ or, equivalently, } C_{\mathrm{M}} = \frac{\rho + \sqrt{\rho^2 - \frac{4Md\log(\epsilon)}{k}}}{2Md}.$$

The last integral in (19), in turn, can be truncated to $[0, C_{\mathrm{j}}]$ where

$$\frac{e^{k\rho C_{\mathrm{j}}}}{e^{kjdC_{\mathrm{j}}^2}} = \epsilon \text{ or, equivalently, } C_{\mathrm{j}} = \frac{\rho + \sqrt{\rho^2 - \frac{4dj\log(\epsilon)}{k}}}{2dj}$$

for the same value of ϵ. Note that:

$$C_{\mathrm{M}} \ll C \text{ for } 1 \ll M \text{ and } C_{\mathrm{j}} \ll C \text{ for } 1 \ll j.$$

To design an efficient way to evaluate the representation given in (19) we need to deal with both the integral involving $f_{\mathrm{M}}(\zeta)$ and those involved in the last term of the representation. Regarding the $f_{\mathrm{M}}(\zeta)$ we first note that:

$$|\int_0^\infty f_{\mathrm{M}}(\zeta)d\zeta| \sim \frac{1}{kMd} \text{ as } k \to \infty$$

and

$$\max|f_{\mathrm{M}}(\zeta)| \sim \frac{e^{k\rho^2/(4Md)}}{\sqrt{\pi kMd}} \text{ and } \max|\frac{df_{\mathrm{M}}}{d\zeta}(\zeta)| \sim e^{\frac{k\rho^2}{4Md}}. \tag{21}$$

To see (21) we look at the behavior of the integrand given in (19). For $\zeta \sim 0$ we have that:

$$k\rho\zeta\sqrt{\zeta^2 - i} \sim k\rho\zeta(1-i),$$

and for fixed $k\rho$

$$J_0(k\rho\zeta\sqrt{\zeta^2 - i}) \sim \sqrt{\frac{2}{\pi k\rho\zeta(1-i)}}e^{ik\rho\zeta(1-i)-i\frac{\pi}{4}}.$$

Therefore:

$$\begin{aligned} f_{\mathrm{M}}(\zeta) &\sim \frac{\zeta}{e^{kMd\zeta^2} - e^{ikMd}}\sqrt{\frac{2}{\pi k\rho\zeta(1-i)}}e^{k\rho\zeta(1+i)-i\frac{\pi}{4}} \\ &\sim \tilde{f}(\zeta) \equiv \sqrt{\frac{2\zeta}{\pi k\rho(1-i)}}\frac{e^{k\rho\zeta(1+i)-i\frac{\pi}{4}}}{e^{kMd(\zeta^2-i)}} \end{aligned} \tag{22}$$

and for large k:

$$\max_{0\le\zeta\le\infty}\left|f_{\mathrm{M}}(\zeta)\right| \sim \frac{e^{k\rho^2/(4Md)}}{\sqrt{\pi kMd}}.$$

Thus a canonical quadrature provides a stable and efficient way to evaluate (19) accurately with a computational complexity independent of the wave number provided:

$$\frac{e^{k\rho^2/(4Md)}}{\sqrt{\pi k M d}} < \frac{\text{constant}}{kMd} \tag{23}$$

where the integrand does not oscillate rapidly within the range $[0, C_{\mathrm{M}}]$. In Figure 1, we display plots of $f_{\mathrm{M}}(\zeta)$ near $\zeta = 0$ and of its logarithm in a larger region for values that satisfy (23).

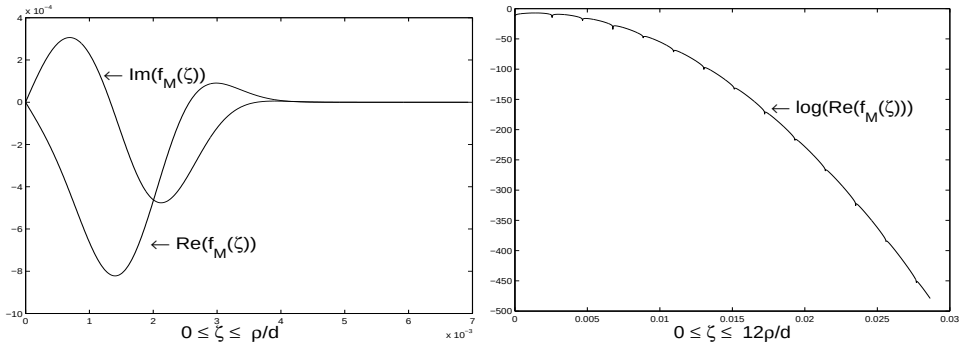

Fig. 1. The integrand $f_{\mathrm{M}}(\zeta)$ in (18) Left: $\Re(f_{\mathrm{M}}(\zeta))$ and $\Im(f_{\mathrm{M}}(\zeta))$, Right: $\log(\Re(f_{\mathrm{M}}(\zeta)))$,with $M = 0$, $k = 10^5 + 0.2$, $d = 2\pi$, $(\rho, z) = (0.015, 0)$ and $k\rho^2/(4d) = 0.89$.

On the other hand and as we anticipated, for large values of $\frac{k\rho^2}{4d}$, the integrand $f_{\mathrm{M}}(\zeta)$ in (19) displays large and fast oscillations which cancel out to produce a significantly smaller integrated value, see Figure 2. Indeed, choosing:

$$\frac{e^{k\rho^2/(4Md)}}{\sqrt{\pi k M d}} > 10^A \frac{1}{kMd} \tag{24}$$

leads to difficulties in attempting to accurately determine the integral value in finite precision arithmetic since a canonical quadrature will lead to a loss of A significant digits in the value of the integral. For the sake of definiteness we shall take:

$$A = 5$$

in double precision arithmetic.

There remains then to design an effective way to evaluate the integral that involves $f_{\mathrm{M}}(\zeta)$ in (19) for values of k and ρ that fall in the regime (24). Fortunately, the first integral in (19) can be treated similarly to its analogue in the case of line arrays [15–17]. Indeed we first note that choosing:

$$M \approx \frac{k\rho^2}{20d}$$

allows us to capture all significant contributions to the integral. With this

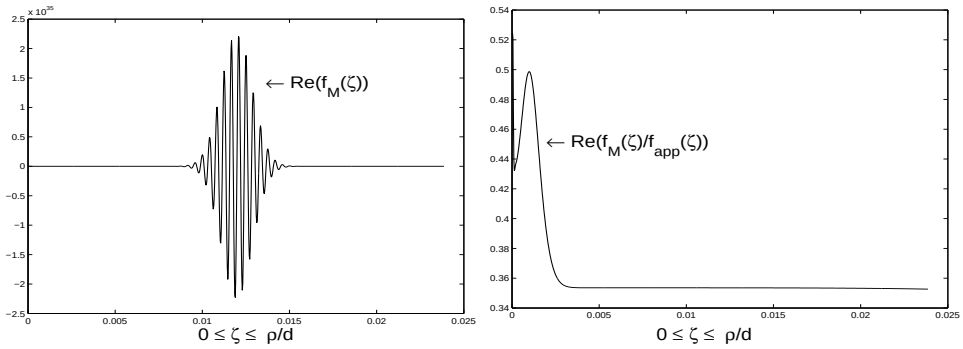

Fig. 2. The integrand $f_{\mathrm{M}}(\zeta)$ in (18) and its approximation $\tilde{f}(\zeta)$ as defined in (22). Left: $\Re(f_{\mathrm{M}}(\zeta))$, Right: $\Re(f_{\mathrm{M}}(\zeta)/\tilde{f}(\zeta))$, with $k = 10^5 + 0.2$, $d = 2\pi$, $(\rho, z) = (0.15, 0)$, and $k\rho^2/(4d) = 89$.

choice of M large variations can be avoided since (see Figure 3):

$$|f_{\mathrm{M}}(\zeta)| \ll |f(\zeta)| \text{ and } |f_{\mathrm{M}}^{'}(\zeta)| \ll |f^{'}(\zeta)|,$$

and a canonical quadrature can be applied to evaluate the integral:

$$\int_0^{C_{\mathrm{M}}} f_{\mathrm{M}}(\zeta) d\zeta$$

accurately with a computational complexity independent of the wave number.

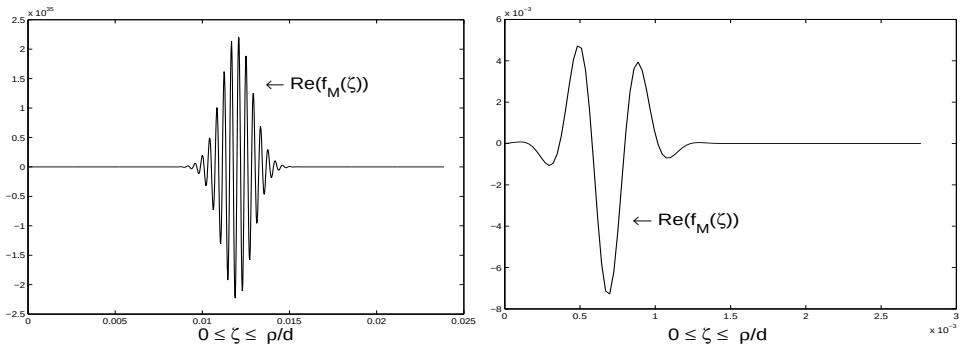

Fig. 3. Real part of the integrand $f_{\mathrm{M}}(\zeta)$ in (18). Left: $M = 0$, Right: $M = 18$ with $k = 10^5 + 0.2$, $d = 2\pi$, $z = 0$, $\rho = 0.15$.

To complete the prescription of our algorithm we need only to device appropriate quadratures in the integrals for the last term of the right hand side of (19). This analysis however *cannot* proceed as in [15,16]. There the basic idea was to construct a quotient of the form:

$$\frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big)}{J_0\Big(k\rho(1-i)\zeta\Big)} = h(\zeta) = \sum_{n=0}^{\infty} a_n \zeta^n \tag{25}$$

to allow for the representation of the integral as:

$$\begin{aligned}\int_0^C \zeta \frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{e^{jkd\zeta^2}} d\zeta &= \int_0^C \zeta \frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{J_0\Big(k\rho(1-i)\zeta\Big)} \frac{J_0(k\rho(1-i)\zeta)}{e^{jkd\zeta^2}} d\zeta \\ &= \sum_{n=0}^{\infty} a_n \int_0^C \zeta^{n+1} \frac{J_0(k\rho(1-i)\zeta)}{e^{jkd\zeta^2}} d\zeta \\ &= \sum_{n=0}^{\infty} a_n I_{n+1,j}^{(0)}\end{aligned} \tag{26}$$

where $I_{n,j}^{(0)}$ is defined by

$$I_{n,j}^{(0)} = \int_0^C \zeta^n \frac{J_0(k\rho(1-i)\zeta)}{e^{jkd\zeta^2}} d\zeta. \tag{27}$$

However, in contrast when compared to the case treated in [15,16], here this procedure is numerically stable only for a much smaller region:

$$k\rho^2/(2d) \leq 1$$

which does not offer any further improvement over the case where classical quadratures are effective. The difficulty arises from the size of the coefficients in (26) when n is small for large $k\rho$. Indeed:

$$\begin{cases} a_{2n} \sim (\frac{k\rho}{2})^{2n-2} \text{ for small } n \text{ and } k\rho \gg 1, \\ a_{2n+1} = 0 \text{ for } n \geq 0. \end{cases}$$

and, as shown below (cf. (39)), the integrals behave like:

$$I_{n+1,j}^{(0)} \sim \frac{i\rho^{2n}}{2^{n+1}k(dj)^{2n+1}} e^{i\frac{k\rho^2}{2jd}} \text{ for } k\rho \gg 1 \text{ and } n \geq 1,$$

so that:

$$a_n I_{n+1,j}^{(0)} \sim (\frac{k\rho^2}{2d})^{2n-2}.$$

As we shall show however a modification of this scheme can be used to derive a stable representation of $J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)$. More precisely, since:

$$\sqrt{\zeta^2-2i} \sim 1-i \text{ for } \zeta \sim 0$$

we can expand:

$$
\begin{aligned}
J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big) &= J_0\Bigg((1-i)k\rho\zeta + \Big[k\rho\zeta\sqrt{\zeta^2-2i}-(1-i)k\rho\zeta\Big]\Bigg) \\
&= \sum_{n=0}^{\infty} \frac{\Big[\zeta\sqrt{\zeta^2-2i}-(1-i)\zeta\Big]^n}{n!}\Bigg(D^n J_0\Bigg)\Big((1-i)k\rho\zeta\Big) \qquad (28)\\
&= \sum_{n=0}^{\infty} \frac{\Big[\zeta\sum_{m=1}^{\infty} r^{2m}\zeta^{2m}\Big]^n}{n!}\Bigg(D^n J_0\Bigg)\Big((1-i)k\rho\zeta\Big)
\end{aligned}
$$

where

$$\sqrt{\zeta^2-2i} = (1-i) + \sum_{m=1}^{\infty} r_{2m}\zeta^{2m} \text{ for } \zeta \leq \sqrt{2}$$

and the coefficients r_{2m} can be easily evaluated via the recursive formula:

$$r_0 = 1-i \text{ and } r_{2m} = \frac{(2m-3)}{2m}\frac{(-1)^{m+1}}{2i}r_{2m-2},\ m = 1,2,...$$

Next, using:

$$D\Bigg(J_0(a)\Bigg) = -J_1(a) \text{ and } D^1\Bigg(J_1(a)\Bigg) = J_0(a) - \frac{J_1(a)}{a},$$

the decomposition in (28) can be rewritten as:

$$J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big) = J_0\Big(k\rho(1-i)\zeta\Big)h_0(\zeta) + J_1\Big(k\rho(1-i)\zeta\Big)h_1(\zeta) \qquad (29)$$

where

$$h_0(\zeta) = \sum_{n=0}^{\infty} b_n\zeta^n \text{ and } h_1(\zeta) = \sum_{n=0}^{\infty} c_n\zeta^n.$$

The coefficients b_n and c_n are explicitly given by

$$
b_{2n} = \begin{cases}
1 & \text{if } n = 0,\\
0 & \text{if } n = 1,2,\\
\sum_{m=1}^{\lfloor \frac{n}{3} \rfloor} \dfrac{(-i)^{n+m}}{2^{n+m}}\dfrac{(n-2m-1)!(n-2m)!}{(n-3m)!(n-m)!}\dfrac{((1-i)k\rho)^{2m}}{m!(m-1)!} & \text{if } n \geq 3,
\end{cases}
$$

and

$$
c_{2n+1} = \begin{cases}
0 & \text{if } n = 0,\\
\sum_{m=1}^{\lfloor \frac{n-1}{3} \rfloor+1} \dfrac{(-i)^{n+m-1}}{2^{n+m}}\dfrac{n-2m+1)!(n-2m+1)!}{(n-3m+2)!(n-m+1)!}\dfrac{((1-i)k\rho)^{2m-1}}{(m-1)!^2} & \text{if } n \geq 1,
\end{cases}
$$

with

$$b_{2n+1} = c_{2n} = 0 \text{ for } n \geq 1$$

and where the "floor function" is defined by $\lfloor x \rfloor = \max\{n \in \mathbb{Z} \ \mid \ x \leq n\}$.

This decomposition provides a more stable way to compute $J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)$ since the coefficients b_n and c_n are smaller than the a_n's in (25)

$$b_{2n} \sim \frac{((1-i)k\rho)^{2\lfloor\frac{n}{3}\rfloor}}{(\frac{2n}{3})!2^{4n/3}} \text{ for } k\rho \gg 1 \text{ and } n \geq 3, \tag{30}$$

$$c_{2n+1} \sim \frac{((1-i)k\rho)^{2\lfloor\frac{n-1}{3}\rfloor+1}}{(\frac{2n}{3})!2^{4n/3}} \text{ for } k\rho \gg 1 \text{ and } n \geq 1. \tag{31}$$

Then, substituting (29) into (17) we obtain:

$$\begin{aligned}\int_0^C \zeta\frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{e^{jkd\zeta^2}}d\zeta &= \sum_{n=0}^{\infty} b_n\left[\int_0^C \zeta^{n+1}\frac{J_0(k\rho(1-i)\zeta)}{e^{jkd\zeta^2}}\,d\zeta\right] \\ &\qquad + \sum_{n=0}^{\infty} c_n\left[\int_0^C \zeta^{n+1}\frac{J_1(k\rho(1-i)\zeta)}{e^{jkd\zeta^2}}\,d\zeta\right] \\ &= \sum_{n=0}^{\infty} b_n I^{(0)}_{n+1,j} + \sum_{n=0}^{\infty} c_n I^{(1)}_{n+1,j} \\ &= \sum_{n=0}^{\infty} b_{2n} I^{(0)}_{2n+1,j} + \sum_{n=1}^{\infty} c_{2n+1} I^{(1)}_{2n+2,j}\end{aligned} \tag{32}$$

where

$$I^{(1)}_{n,j} = \int_0^C \zeta^n \frac{J_1\Big(k\rho(1-i)\zeta\Big)}{e^{jkd\zeta^2}}d\zeta$$

and $I^{(0)}_{n,j}$ is as in (27).

The evaluation of the integrals $I^{(0)}_{2n+1,j}$ and $I^{(1)}_{2n,j}$ in (32) is clearly preferable to that in (14), on account of the diminishing values and faster decay of the former as j increases. Moreover, as we show next, $I^{(0)}_{2n+1,j}$ and $I^{(1)}_{2n,j}$ can be computed explicitly, with the use of Hankel's formula [18]:

$$\int_0^\infty \zeta^{\mu-1}\frac{J_\nu\Big(a\zeta\Big)}{e^{p^2\zeta^2}}\,d\zeta = \frac{\Gamma(\frac{1}{2}\nu+\frac{1}{2}\mu)(\frac{1}{2}a/p)^\nu}{2p^\mu\Gamma(\nu+1)}\,{}_1F_1(\frac{1}{2}\nu+\frac{1}{2}\mu;\nu+1;-\frac{a^2}{4p^2}), \text{ if } \Re(\mu+\nu)>0, \tag{33}$$

where ${}_1F_1$ denotes the confluent hypergeometric function of the first kind.

To this end we will first consider the evaluation of $I^{(0)}_{2n+1,j}$ and let:

$$V^{(0)}_{2n+1,j} = \int_0^\infty \zeta^{2n+1}\frac{J_0\Big(k\rho(1-i)\zeta\Big)}{e^{kdu^2}}d\zeta.$$

Then from (33) (with $\nu = 0$ and $\mu = 2n+2$):

$$V^{(0)}_{2n+1,j} = \frac{\Gamma(n+1)}{2(kdj)^{n+1}} {}_1F_1(n+1, 1; \frac{ik\rho^2}{2dj}) \tag{34}$$

where for fixed b the hypergeometric function ${}_1F_1(n, b; \frac{ik\rho^2}{2dj})$ can be evaluated through the recursive formula [12, Eq. 13.4.1]

$${}_1F_1(a+1, b, c) = \frac{(c+2a-b)}{a} {}_1F_1(a, b, c) + \frac{(b-a)}{a} {}_1F_1(a-1, b, c), \tag{35}$$

with

$${}_1F_1(b, b; c) = e^c \text{ and } {}_1F_1(b+1, b; c) = \frac{(c+b)}{b}, \tag{36}$$

and with $b = 1$. Alternatively ${}_1F_1(n, 1; \frac{ik\rho^2}{2dj})$ can be evaluated explicitly as:

$${}_1F_1(n+b, b; \frac{ik\rho^2}{2dj}) = e^{i\frac{k\rho^2}{2dj}} \sum_{m=0}^{n} \frac{n!}{m!(n-m)!(n-m+b-1)!} (i\frac{k\rho^2}{2dj})^{n-m}.$$

As we shall see $V^{(0)}_{2n+1,j}$ provides a good approximation to $I^{(0)}_{2n+1,j}$ for n small. For n large, on the other hand, it follows from (34) that:

$$V^{(0)}_{2n+1,j} \to \infty \text{ as } n \to \infty$$

and these values do not provide a good estimate of $I^{(0)}_{2n+1,j}$. However, in this case, we can simply estimate:

$$|I^{(0)}_{n,j}| < \epsilon C^{n+1} \text{ for } n > N,$$

where ϵ is as in (20), provided:

$$N = \frac{k\rho^2}{8d} - \frac{\log(\epsilon)}{2} + \frac{k\rho}{4d}\sqrt{\rho^2 - \frac{4d\log(\epsilon)}{k}}.$$

Given such N then we have:

$$|I^{(0)}_{n,j} - V^{(0)}_{n,j}| \leq \epsilon C^n \text{ for } n \leq N.$$

A similar argument delivers:

$$|I^{(1)}_{n,j}| < \epsilon C^{n+1} \text{ for } n > N,$$

and

$$|I^{(1)}_{n,j} - V^{(1)}_{n,j}| \leq \epsilon C^n \text{ for } n \leq N,$$

where

$$V_{2n,j}^{(1)} = \int_0^\infty \zeta^{2n} \frac{J_1\Big(k\rho(1-i)\zeta\Big)}{e^{kdu^2}} d\zeta.$$

As before, from (33) ($\nu = 1$ and $\mu = 2n+3$), we have:

$$V_{2n,j}^{(1)} = \frac{\Gamma(n+2)(k\rho(1-i))}{4(kdj)^{n+2}} {}_1F_1(n+2, 2; \frac{ik\rho^2}{2dj}) \tag{37}$$

where ${}_1F_1(n, 2; \frac{ik\rho^2}{2dj})$ can again be calculated through (35) and (36) (with $b = 2$).

Finally using (34) and (37) the Green function $G(\rho, 0)$ can be written as:

$$\begin{aligned} G(\rho, 0) \approx & \frac{e^{ik\rho}}{4\pi\rho} + \frac{k}{\pi} \int_0^{C_{\mathrm{M}}} f_{\mathrm{M}}(\zeta)\, d\zeta \\ & + \frac{k}{\pi} \sum_{j=1}^{M} e^{ikjd} \sum_{n=0}^{N} b_{2n} \frac{n!}{2(kdj)^{n+1}} {}_1F_1(n+1, 1; \frac{ik\rho^2}{2dj}) \\ & + \frac{k}{\pi} \sum_{j=1}^{M} e^{ikjd} \sum_{n=1}^{N} c_{2n+1} \frac{(n+1)!(k\rho(1-i))}{4(kdj)^{n+2}} {}_1F_1(n+2, 2; \frac{ik\rho^2}{2dj}). \end{aligned} \tag{38}$$

To see that (38) improves on the stability of a direct application of (14) we first note that:

$$\frac{n!}{2(kdj)^{n+1}} {}_1F_1(n+1, 1; \frac{ik\rho^2}{2dj}) \sim \frac{i\rho^{2n} e^{i\frac{k\rho^2}{2jd}}}{2^{n+1} k (dj)^{2n+1}} \text{ for } k\rho \gg 1 \text{ and } n \geq 1, \tag{39}$$

and using (30), the terms in the first inner sum decay as:

$$\left| b_{2n} \frac{n!}{2(kdj)^{n+1}} {}_1F_1(n+1, 1; \frac{ik\rho^2}{2dj}) \right| \sim \frac{1}{2kdj} \left(\frac{k\rho^4}{8\sqrt{2}(dj)^3} \right)^{2n/3} \frac{1}{(2n/3)!} \text{ for } n \geq 1. \tag{40}$$

A similar argument applies to the second inner sum in (38). In this case:

$$\frac{(n+1)!(k\rho(1-i))}{4(kdj)^{n+2}} {}_1F_1(n+2, 2; \frac{ik\rho^2}{2dj}) \sim \frac{(1+i)\rho^{2n-1} e^{i\frac{k\rho^2}{2jd}}}{2^{n+1} k (dj)^{2n}} \text{ for } k\rho \gg 1 \text{ and } n \geq 1,$$

and, using (31), we see that:

$$\left| c_{2n+1} \frac{(n+1)!(k\rho(1-i))}{4(kdj)^{n+2}} {}_1F_1(n+2, 2; \frac{ik\rho^2}{2dj}) \right| \sim \frac{1}{2(k\rho)^{2/3}} \left(\frac{k\rho^4}{16 d^3 j^3} \right)^{2n/3} \text{ for } n \geq 1. \tag{41}$$

Finally we note that, for stability, (40) and (41) demand only that:

$$\frac{k\rho^4}{d^3} < \text{ constant}$$

which significantly improves upon (14); see Tables 5– 8.

5 Extension to partial derivatives of $G(\rho, z)$

Beyond that of $G(\rho, z)$ the solution of the scattering problem typically necessitates the evaluation of its normal derivatives (e.g. in connection with integral equations that rely on double layer potential –or derivatives of single layer potential– representations). In this section we show that the derivations in §2 and §3 largely extend to this latter case resulting in efficient mechanisms for the numerical evaluation of the partial derivatives of $G(\rho, z)$. More precisely, we have the representations:

1. <u>Spatial representation:</u> By taking the partial derivatives of the basic representation in (1), one can easily derive:

$$\frac{\partial G}{\partial \rho}(\rho, z) = \frac{\rho}{4\pi} \sum_{n=-\infty}^{\infty} e^{i\alpha nd} \frac{e^{ikr_n}}{r_n^2} \left(ik - \frac{1}{r_n} \right) \tag{42}$$

and

$$\frac{\partial G}{\partial z}(\rho, z) = \frac{1}{4\pi} \sum_{n=-\infty}^{\infty} (z - nd) e^{i\alpha nd} \frac{e^{ikr_n}}{r_n^2} \left(ik - \frac{1}{r_n} \right) \tag{43}$$

An analysis similar to that in (2) above shows that terms in (42) decay as $\frac{1}{n^2}$ while those in (43) decay as $\frac{1}{n}$. For N large, we thus have:

$$\begin{aligned} \left| \frac{\partial G}{\partial \rho}(\rho, z) - \frac{\rho}{4\pi} \sum_{n=-N}^{N} e^{i\alpha nd} \frac{e^{ikr_n}}{r_n^2} \left(ik - \frac{1}{r_n} \right) \right| &\approx \left| \frac{i\rho k}{2\pi} \frac{e^{i(N+1)(k+\alpha)d}}{(N+1)^2 d^2} \right| \\ &= \frac{k\rho}{2\pi (N+1)^2 d^2} \end{aligned} \tag{44}$$

and

$$\begin{aligned} \left| \frac{\partial G}{\partial \rho}(\rho, z) - \frac{1}{4\pi} \sum_{n=-N}^{N} (z - nd) e^{i\alpha nd} \frac{e^{ikr_n}}{r_n^2} \left(ik - \frac{1}{r_n} \right) \right| &\approx \left| \frac{ik}{2\pi} \frac{e^{i(N+1)(k+\alpha)d}}{(N+1)d} \right| \\ &= \frac{k}{2\pi (N+1)d}. \end{aligned} \tag{45}$$

2. <u>Spectral representation:</u> Using the spectral representation given by (4), one can derive:

$$\frac{\partial G}{\partial \rho}(\rho, z) = \frac{1}{4id} \sum_{n=-\infty}^{\infty} \beta_n e^{i\alpha_n z} H_1^{(1)}(\beta_n \rho),$$

and

$$\frac{\partial G}{\partial z}(\rho,z) = -\frac{1}{4d}\sum_{n=-\infty}^{\infty} \alpha_n e^{i\alpha_n z} H_0^{(1)}(\beta_n \rho);$$

the series here can be truncated exactly as in (5).

3. <u>Integral representation:</u> Finally, partial derivatives for the new integral representations are given by

$$\begin{aligned}\frac{\partial G}{\partial \rho}(\rho,z) = \frac{\rho}{4\pi}\frac{e^{ikr_0}}{r_0^2}\left(ik-\frac{1}{r_0}\right) - \frac{k^2}{\pi}\Bigg[\int_0^\infty f^{(+_\rho)}(\zeta)d\zeta + \int_0^\infty f^{(-_\rho)}(\zeta)d\zeta \\ + \sum_{j=1}^{M} e^{ikz+i(k+\alpha)dj}\int_0^\infty \zeta^2\sqrt{\zeta^2-2i}\frac{J_1\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{e^{k\zeta^2(dj+z)}}d\zeta \\ + \sum_{j=1}^{M} e^{-ikz+i(k-\alpha)dj}\int_0^\infty \zeta^2\sqrt{\zeta^2-2i}\frac{J_1\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{e^{k\zeta^2(dj-z)}}d\zeta\Bigg]\end{aligned}$$

where

$$f^{(\pm_\rho)}(\zeta) = \zeta^2\sqrt{\zeta^2-2i}\frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha(M+1)d}e^{(M+1)kd(\zeta^2-i)} - e^{\pm i\alpha Md}e^{Mkd(\zeta^2-i)}}J_1\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)$$

and

$$\begin{aligned}\frac{\partial G}{\partial z}(\rho,z) = \frac{z}{4\pi}\frac{e^{ikr_0}}{r_0^2}\left(ik-\frac{1}{r_0}\right) - \frac{k}{2\pi}\Bigg[\int_0^\infty f^{(+_z)}(\zeta)d\zeta + \int_0^\infty f^{(-_z)}(\zeta)d\zeta \\ + \sum_{j=1}^{M} e^{ikz+i(k+\alpha)dj}\int_0^\infty k(i-\zeta^2)\zeta\frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{e^{k\zeta^2(dj+z)}}d\zeta \\ + \sum_{j=1}^{M} e^{-ikz+i(k-\alpha)dj}\int_0^\infty k(-i+\zeta^2)\zeta\frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{e^{k\zeta^2(dj-z)}}d\zeta\Bigg]\end{aligned}$$

where

$$f^{(\pm_z)}(\zeta) = (\mp ik \pm k\zeta^2)\zeta\frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha(M+1)d}e^{(M+1)kd(\zeta^2-i)} - e^{\pm i\alpha Md}e^{Mkd(\zeta^2-i)}}J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big).$$

Here the integrals can be truncated exactly as those corresponding to $G(\rho,z)$ in (20).

6 Set of numerical results

In this section, we provide three sets of numerical experiments where we compare the values and computational times associated with the Green function $G(\rho,z) = G(x,y,z)$ and its partial derivatives obtained from the new integral

representation (38), the classical spatial and spectral representations (cf. (1), (4)), and the Ewald's transform (6). More precisely the first two of these sets correspond to the Green function itself when $k\rho^2/(4d) \lesssim 1$ and $1 \ll k\rho^2/(4d)$, respectively, and the last set to its partial derivatives.

The implementation of every scheme is largely straightforward, as it entails evaluations of standard special functions and simple sums and products. For the Ewald method the necessary evaluations of the complementary error function – for complex arguments – are performed using the algorithm in [19]. The method introduced in §4 and §5, on the other hand, relies on the evaluation of integrals (cf. I^M_{new} in (18)) with integrands that display exponentially small (odd order) derivatives at the boundary of the integration domain and are thus amenable to very accurate evaluations via the trapezoidal rule.

For comparison purposes, and to enhance accuracy, all calculations were performed in double precision arithmetic. For the evaluation of the relative error of the Green function:

$$\text{Err} = \frac{|G^{\text{Exa.}}(\rho, z) - G^{\text{Eva.}}(\rho, z)|}{|G^{\text{Exa.}}(\rho, z)|}, \tag{46}$$

and that of its partial derivatives:

$$\text{Err}_\rho = \frac{|\frac{\partial G^{\text{Exa.}}}{\partial \rho}(\rho, z) - \frac{\partial G^{\text{Eva.}}}{\partial \rho}(\rho, z)|}{|\frac{\partial G^{\text{Exa.}}}{\partial \rho}(\rho, z)|} \text{and } \text{Err}_{\text{z}} = \frac{|\frac{\partial G^{\text{Exa.}}}{\partial z}(\rho, z) - \frac{\partial G^{\text{Eva.}}}{\partial z}(\rho, z)|}{|\frac{\partial G^{\text{Exa.}}}{\partial z}(\rho, z)|} \tag{47}$$

an "exact solution" for $G^{\text{Exa.}}(\rho, z)$, $\frac{\partial G^{\text{Exa.}}}{\partial \rho}(\rho, z)$ and $\frac{\partial G^{\text{Exa.}}}{\partial z}(\rho, z)$ was computed in quadruple precision arithmetic (using the spectral representation to avoid biases). The tables confirm the expected behavior of each methodology, as discussed above.

In Tables 1-10, the sums in the spatial representation were truncated at $\text{N}_5 = 10^5$ and $\text{N}_6 = 10^6$ to display the first order convergence demonstrated in (2). Truncation for the spectral representation, on the other hand, is based on the exponential convergence of the method. The Ewald transformation, on the other hand, displays a stronger instability, enhanced for increasing ρ, as the values of the wave number exceed the ratio $\max\{\sqrt{\rho^2 + z^2}/\rho^2, 1/\rho\}$ (cf. (12)). The cases where this method does not converge ("dnc") are labeled as such.

In Tables 11-14, on the other hand, the sum in the spatial representation for ρ derivative are truncated for $\text{N}_1 = 10$ and $\text{N}_2 = 10^2$, since as we explained in (44) the convergence here is quadratic. Sums in the spatial representation for the z derivatives are again truncated at $\text{N}_5 = 10^5$ and $\text{N}_6 = 10^6$ as convergence

for these is only linear (45), similar to that of $G(\rho, z)$ itself. Truncation for the spectral representation is again based on the exponential convergence of the method.

In the first set of the numerical experiments Tables 1-4, we consider the case where $z = 0.1$ for $\rho = 0.001$ and $\rho = \sqrt{d/k}$ leading to values $k\rho^2/(4d) \lesssim 1$. Here $\alpha = 0$, in Tables 1-2 and $\alpha = k\sin(\frac{\pi}{3})$, in Tables 3-4. In the second set, we let $\alpha = 0$, $z = 0$ for $\rho = 0.01, 0.1, 0.3$ and $\rho = 0.5$, in Tables 5-8, and we let $(\rho, z) = (0.1, 0.1)$ for $\alpha = k/\sin(\frac{\pi}{3})$ and $\alpha = k/\sin(\frac{\pi}{6})$, in Tables 9-10, all of which lead to values $1 \ll k\rho^2/(4d)$. In the third set Tables 11-14, we consider the case where, $z = 0.1$ for $\rho = 0.001$ and $\rho = \sqrt{d/k}$. In all numerical experiments we let the period $d = 2\pi$.

As the tables show, the schemes introduced here can be seen to consistently outperform the alternative procedures within its domain of applicability, where it delivers higher accuracy in shorter computational times.

Table 1
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $\alpha = 0,\ k = 10^n + 0.2,\ (\rho, z) = (0.001, 0.1)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	1.4e-7	0.3s	1.4e-8	3s	3.8e-15	5s	1.9e-16	0.1s	1.9e-16	0.2s
2	2.2e-7	0.3s	2.2e-8	3s	6.9e-15	5s	5.8e-14	0.2s	1.1e-15	0.2s
3	2.4e-7	0.3s	2.4e-8	3s	9.5e-15	5s	1.1e-13	2s	4.6e-15	0.2s
4	1.4e-7	0.3s	1.4e-8	3s	2.0e-13	5s	4.8e-13	40s	2.0e-13	0.2s
5	2.5e-7	0.3s	2.5e-8	3s	7.5e-13	17s	dnc	...	6.7e-12	0.2s
6	2.7e-7	0.3s	2.7e-8	3s	9.1e-12	163s	dnc	...	3.4e-11	0.2s
7	2.6e-7	0.3s	2.6e-8	3s	1.2e-10	1648s	dnc	...	2.3e-10	0.2s

Table 2
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $\alpha = 0,\ k = 10^n + 0.2,\ (\rho, z) = (\sqrt{d/k}, 0.1)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	9.9e-7	0.3s	9.9e-8	3s	1.3e-15	0.1s	1.1e-13	0.1s	2.0e-15	0.2s
2	6.6e-7	0.3s	6.6e-8	3s	3.4e-15	0.1s	dnc	...	1.0e-15	0.2s
3	2.9e-7	0.3s	2.9e-8	3s	1.1e-14	0.2s	dnc	...	5.6e-15	0.2s
4	1.5e-7	0.3s	1.5e-8	3s	1.3e-13	1.6s	dnc	...	1.8e-13	0.2s
5	2.5e-7	0.3s	2.5e-8	3s	1.2e-12	16s	dnc	...	1.2e-12	0.2s
6	2.7e-7	0.3s	2.7e-8	3s	1.0e-11	163s	dnc	...	3.1e-11	0.2s
7	2.6e-7	0.3s	2.6e-8	3s	1.0e-10	1645s	dnc	...	3.3e-10	0.2s

Table 3
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $\alpha = k\sin(\frac{\pi}{3}),\ k = 10^n + 0.2,\ (\rho, z) = (0.001, 0.1)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	7.1e-07	0.5s	7.6e-08	5s	1.0e-14	7s	2.1e-14	0.1s	1.8e-15	0.2s
2	1.1e-06	0.5s	1.1e-07	5s	2.0e-14	7s	2.9e-12	0.4s	6.7e-16	0.2s
3	1.7e-05	0.5s	1.7e-06	5s	5.5e-13	7s	5.6e-13	4s	6.3e-13	0.2s
4	1.7e-07	0.5s	4.3e-09	5s	1.2e-13	7s	9.3e-13	110s	1.8e-13	0.2s
5	3.4e-07	0.5s	3.5e-08	5s	2.6e-12	30s	dnc	...	2.6e-12	0.2s
6	2.0e-07	0.5s	2.2e-08	5s	1.6e-11	275s	dnc	...	1.2e-11	0.2s
7	2.1e-06	0.5s	2.5e-07	5s	5.6e-10	2900s	dnc	...	2.8e-10	0.2s

Table 4
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $\alpha = k\sin(\frac{\pi}{3}),\ k = 10^n + 0.2,\ (\rho, z) = (\sqrt{d/k}, 0.1)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	6.2e-06	0.5s	6.6e-07	5s	1.1e-14	0.1s	1.4e-13	0.2s	1.8e-14	0.2s
2	2.6e-06	0.5s	2.7e-07	5s	3.1e-15	0.1s	dnc	...	5.7e-15	0.2s
3	2.4e-05	0.5s	2.4e-06	5s	8.2e-13	0.3s	dnc	...	9.2e-13	0.2s
4	1.7e-07	0.5s	4.4e-09	5s	1.5e-13	3s	dnc	...	2.6e-13	0.2s
5	3.3e-07	0.5 s	3.4e-08	5s	1.1e-12	27s	dnc	...	7.1e-12	0.2s
6	2.0e-07	0.5 s	2.0e-08	5s	1.9e-11	278s	dnc	...	2.1e-11	0.2s
7	2.2e-06	0.5 s	2.3e-07	5s	5.7e-10	2850s	dnc	...	2.6e-10	0.2s

Table 5
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $\alpha = 0, k = 10^n + 0.2, (\rho, z) = (0.01, 0)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	2.7e-08	0.3s	2.7e-09	3s	4.1e-15	0.5s	1.1e-15	0.1s	1.1e-16	0.2s
2	2.7e-08	0.3s	2.7e-09	3s	1.2e-15	0.5s	2.8e-12	0.2s	1.1e-16	0.2s
3	2.7e-08	0.3s	2.7e-09	3s	4.8e-15	0.5s	1.3e-10	2s	9.0e-16	0.2s
4	2.7e-08	0.3s	2.7e-09	3s	1.2e-14	1s	dnc	...	9.8e-15	0.2s
5	2.7e-08	0.3s	2.6e-09	3s	1.0e-13	9s	dnc	...	8.4e-14	0.2s
6	2.7e-08	0.3s	2.5e-09	3s	1.5e-12	89s	dnc	...	5.6e-12	0.2s
7	2.7e-08	0.3s	2.5e-09	3s	1.5e-12	890s	dnc	...	5.6e-12	0.2s

Table 6
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $\alpha = 0, k = 10^n + 0.2, (\rho, z) = (0.1, 0)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	2.6e-07	0.3s	3s	2.6e-08	8.9e-16	0.5s	2.0e-14	0.1s	4.3e-16	0.2s
2	2.7e-07	0.3s	3s	2.7e-08	1.4e-15	0.5s	1.7e-12	0.1s	1.6e-15	0.2s
3	2.8e-07	0.3s	3s	2.8e-08	4.2e-15	0.5s	dnc	...	3.4e-15	0.2s
4	2.6e-07	0.3s	3s	2.6e-08	5.7e-13	1s	dnc	...	8.7e-14	0.2s
5	2.7e-07	0.3s	3s	2.7e-08	1.4e-12	9s	dnc	...	7.1e-13	0.2s
6	2.7e-07	0.3s	3s	2.4e-08	3.9e-11	85s	dnc	...	1.5e-10	0.4s

Table 7
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $\alpha = 0, k = 10^n + 0.2, (\rho, z) = (0.3, 0)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	7.8e-07	0.3s	7.8e-08	3s	2.2e-16	0.1s	4.5e-14	0.1s	1.1e-15	0.2s
2	8.8e-07	0.3s	8.8e-08	3s	4.8e-15	0.1s	dnc	...	4.7e-15	0.2s
3	8.9e-07	0.3s	8.9e-08	3s	2.8e-14	0.1s	dnc	...	5.0e-14	0.2s
4	7.7e-07	0.3s	7.7e-08	3s	2.4e-12	1s	dnc	...	3.9e-13	0.2s
5	8.3e-07	0.3s	8.1e-08	3s	3.1e-11	10s	dnc	...	3.5e-11	0.6s
6	7.5e-07	0.3s	8.2e-08	3s	4.6e-10	100s	dnc	...	1.0e-02	2s

Table 8
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $\alpha = 0, k = 10^n + 0.2, (\rho, z) = (0.5, 0)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	1.6e-06	0.3s	1.6e-07	3s	2.1e-16	0.1s	3.4e-14	0.1s	1.2e-15	0.2s
2	1.6e-06	0.3s	1.6e-07	3s	7.7e-15	0.1s	dnc	...	1.6e-14	0.2s
3	1.2e-06	0.3s	1.2e-07	3s	3.5e-14	0.1s	dnc	...	9.4e-14	0.2s
4	1.3e-06	0.3s	1.3e-07	3s	6.1e-12	1s	dnc	...	2.5e-12	0.2s
5	1.5e-06	0.3s	1.4e-07	3s	8.4e-11	9s	dnc	...	1.3e-03	0.6s
6	1.2e-06	0.3s	1.2e-07	3s	8.5e-10	95s	dnc	...	3.7e+07	7s

Table 9
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $k = 10^n + 0.2, \alpha = k/\sin(\frac{\pi}{3}), (\rho, z) = (0.1, 0.1)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	1.8e-006	0.5s	1.8e-007	5s	4.1e-016	0.2s	1.6e-014	0.5s	1.6e-015	0.4s
2	4.0e-007	0.5s	4.4e-008	5s	4.3e-015	0.2s	3.4e-013	2s	1.1e-014	0.4s
3	3.3e-007	0.5s	4.0e-008	5s	2.2e-014	0.4s	dnc	...	6.4e-014	0.4s
4	1.0e-006	0.5s	1.0e-007	5s	6.7e-013	2.5s	dnc	...	6.8e-013	0.4s
5	3.9e-007	0.5s	4.2e-008	5s	3.4e-012	24s	dnc	...	1.1e-011	0.4s
6	1.2e-006	0.5s	1.2e-007	5s	1.9e-011	250s	dnc	...	2.0e-010	0.4s

Table 10
Error (46) and computational times (t) for evaluation of $G(\rho, z)$ with $k = 10^n + 0.2, \alpha = k/\sin(\frac{\pi}{6}), (\rho, z) = (0.1, 0.1)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	Ewa.	$t_{Ewa.}$	NA	t_{NA}
1	1.0e-007	0.5s	1.0e-008	5s	1.0e-015	0.2s	1.5e-014	0.5s	4.8e-016	0.4s
2	1.9e-007	0.5s	1.9e-008	5s	4.0e-015	0.2s	3.5e-013	2s	8.2e-015	0.4s
3	3.0e-007	0.5s	3.2e-008	5s	6.7e-015	0.4s	dnc	...	2.9e-014	0.4s
4	1.0e-007	0.5s	1.2e-008	5s	2.1e-012	2.5s	dnc	...	1.6e-012	0.4s
5	2.4e-007	0.5s	9.6e-008	5s	1.1e-012	27s	dnc	...	5.3e-012	0.4s
6	3.6e-007	0.5s	3.5e-006	5s	9.0e-011	272s	dnc	...	4.0e-010	0.4s

Table 11
Error (46) and computational times (t) for evaluation of $\frac{\partial G}{\partial \rho}(\rho, z)$ with $\alpha = 0, k = 10^n + 0.2, (\rho, z) = (0.001, 0.1)$.

n	Spa.	$t^{N_1}_{Spa.}$	Spa.	$t^{N_2}_{Spa.}$	Spe.	$t_{Spe.}$	NA	t_{NA}
1	1.4e-006	<0.001s	1.5e-008	<0.001s	1.0e-012	5s	6.1e-016	0.2s
2	3.1e-006	<0.001s	3.5e-008	<0.001s	1.8e-013	5s	1.4e-015	0.2s
3	3.3e-006	<0.001s	3.7e-008	<0.001s	1.0e-013	5s	1.2e-014	0.2s
4	2.0e-006	<0.001s	2.3e-008	<0.001s	2.0e-013	5s	2.1e-013	0.2s
5	3.6e-006	<0.001s	4.0e-008	<0.001s	2.0e-012	21s	4.8e-013	0.2s
6	3.8e-006	<0.001s	4.2e-008	<0.001s	1.7e-012	2105s	9.7e-012	0.2s
7	3.6e-006	<0.001s	4.0e-008	<0.001s	3.3e-011	2125s	1.3e-011	0.2s

Table 12
Error (46) and computational times (t) for evaluation of $\frac{\partial G}{\partial z}(\rho, z)$ with $\alpha = 0, k = 10^n + 0.2, (\rho, z) = (0.001, 0.1)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	NA	t_{NA}
1	1.6e-007	0.3s	1.6e-008	3s	2.9e-014	5s	4.8e-016	0.2s
2	1.5e-007	0.3s	1.5e-008	3s	1.6e-014	5s	1.3e-015	0.2s
3	1.3e-007	0.3s	1.3e-008	3s	1.4e-014	5s	1.0e-014	0.2s
4	2.3e-007	0.3s	2.3e-008	3s	6.8e-014	5s	2.1e-013	0.2s
5	8.8e-008	0.3s	9.0e-009	3s	4.8e-013	21s	7.0e-013	0.2s
6	3.5e-009	0.3s	8.5e-010	3s	1.9e-012	210s	8.9e-012	0.2s
7	8.4e-008	0.3s	1.0e-008	3s	3.6e-011	2125s	9.9e-011	0.2s

Table 13
Error (46) and computational times (t) for evaluation of $\frac{\partial G}{\partial \rho}(\rho, z)$ with $\alpha = 0, k = 10^n + 0.2, (\rho, z) = (\sqrt{d/k}, 0.1)$.

n	Spa.	$t^{N_1}_{Spa.}$	Spa.	$t^{N_2}_{Spa.}$	Spe.	$t_{Spe.}$	NA	t_{NA}
1	1.2e-004	<0.001s	1.3e-006	<0.001s	5.3e-016	0.2s	1.7e-015	0.2s
2	2.3e-005	<0.001s	2.5e-007	<0.001s	4.3e-015	0.2s	6.9e-015	0.2s
3	5.4e-006	<0.001s	6.0e-008	<0.001s	7.2e-015	0.3s	3.4e-015	0.2s
4	2.2e-006	<0.001s	2.4e-008	<0.001s	1.4e-013	1.7s	1.8e-013	0.2s
5	3.6e-006	<0.001s	4.0e-008	<0.001s	4.4e-013	21s	5.3e-013	0.2s
6	3.8e-006	<0.001s	4.2e-008	<0.001s	3.2e-012	213s	1.5e-012	0.2s
7	3.6e-006	<0.001s	4.0e-008	<0.001s	1.3e-010	2131s	3.6e-011	0.2s

Table 14
Error (46) and computational times (t) for evaluation of $\frac{\partial G}{\partial z}(\rho, z)$ with $\alpha = 0, k = 10^n + 0.2, (\rho, z) = (\sqrt{d/k}, 0.1)$.

n	Spa.	$t^{N_5}_{Spa.}$	Spa.	$t^{N_6}_{Spa.}$	Spe.	$t_{Spe.}$	NA	t_{NA}
1	8.3e-006	0.3s	8.3e-007	3s	2.9e-015	0.2s	9.7e-015	0.2s
2	1.0e-006	0.3s	1.0e-007	3s	6.6e-015	0.2s	4.7e-015	0.2s
3	2.1e-007	0.3s	2.1e-008	3s	9.2e-015	0.3s	4.5e-015	0.2s
4	2.4e-007	0.3s	2.4e-008	3s	1.2e-013	1.7s	1.9e-013	0.2s
5	8.9e-008	0.3s	8.8e-009	3s	4.7e-013	21s	7.3e-013	0.2s
6	3.8e-009	0.3s	4.2e-010	3s	1.7e-012	213s	1.8e-012	0.2s
7	8.8e-008	0.3s	9.2e-009	3s	2.9e-011	2131s	9.6e-011	0.2s

Appendix A: Formulation of the new algorithm for arbitrary incidence and evaluation points

In this appendix we provide the details on the extension of the formulas (19)–(38) to the most general case $\alpha \in \mathbb{R}$ and $-d/2 \leq z \leq d/2$. For this we look at the integral representation given by (13):

$$G(\rho, z) = \frac{1}{4\pi}\frac{e^{ikr_0}}{r_0} + \frac{k}{2\pi}\Big[\int_0^\infty f^+(\zeta)d\zeta + \int_0^\infty f^-(\zeta)d\zeta\Big]$$

where

$$f^+(\zeta) = \zeta\frac{e^{ikz}e^{-kz\zeta^2}}{e^{i\alpha d}e^{kd(\zeta^2-i)} - 1}J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big)d\zeta,$$
$$f^-(\zeta) = \zeta\frac{e^{-ikz}e^{kz\zeta^2}}{e^{-i\alpha d}e^{kd(\zeta^2-i)} - 1}J_0\Big(k\rho\zeta\sqrt{\zeta^2 - 2i}\Big)d\zeta,$$

note that for $\alpha = 0$ and $z = 0$, we have $f^+(\zeta) = f^-(\zeta)$. For the evaluation of the Green function to the most general case we proceed as in (16)-(32), and truncate the integrals to intervals:

$$C^\pm = \frac{\rho + \sqrt{\rho^2 - \frac{4(d\pm z)\log(\epsilon)}{k}}}{2(d \pm z)}$$

to derive:

$$\begin{aligned}
\int_0^{C^\pm} f^\pm(\zeta)d\zeta &= \int_0^{C^\pm} \zeta \frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha d}e^{kd(\zeta^2-i)}-1} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&= \int_0^{C^\pm} \zeta \frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha(M+1)d}e^{(M+1)kd(\zeta^2-i)}-e^{\pm i\alpha Md}e^{Mkd(\zeta^2-i)}} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&\quad + \sum_{j=1}^{M}\int_0^{C^+} \zeta \frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha dj}e^{kdj(\zeta^2-i)}} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&= \int_0^{C^\pm} \zeta \frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha(M+1)d}e^{(M+1)kd(\zeta^2-i)}-e^{\pm i\alpha Md}e^{Mkd(\zeta^2-i)}} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&\quad + \sum_{j=1}^{M} e^{ikz+i(k\mp\alpha)dj}\int_0^{\infty} \zeta \frac{J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)}{e^{k\zeta^2(dj\pm z)}}d\zeta
\end{aligned}$$

Moreover from this:

$$\begin{aligned}
\int_0^{C^\pm} f^\pm(\zeta)d\zeta &= \int_0^{C^\pm} \zeta \frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha(M+1)d}e^{(M+1)kd(\zeta^2-i)}-e^{\pm i\alpha Md}e^{Mkd(\zeta^2-i)}} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&\quad + \sum_{j=1}^{M} e^{ikz+i(k\mp\alpha)dj}\sum_{n=0}^{\infty} b_n\left[\int_0^{C} \zeta^{n+1}\frac{J_0(k\rho(1-i)\zeta)}{e^{k\zeta^2(dj\pm z)}}d\zeta\right] \\
&\quad + \sum_{j=1}^{M} e^{ikz+i(k\mp\alpha)dj}\sum_{n=0}^{\infty} c_n\left[\int_0^{C} \zeta^{n+1}\frac{J_1(k\rho(1-i)\zeta)}{e^{k\zeta^2(dj\pm z)}}d\zeta\right] \\
&= \int_0^{C^\pm} \zeta \frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha(M+1)d}e^{(M+1)kd(\zeta^2-i)}-e^{\pm i\alpha Md}e^{Mkd(\zeta^2-i)}} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&\quad + \sum_{j=1}^{M} e^{ikz+i(k\mp\alpha)dj}\sum_{n=0}^{\infty} b_n I_{n+1,j}^{(0,z,\pm)} + \sum_{j=1}^{M} e^{ikz+i(k\mp\alpha)dj}\sum_{n=0}^{\infty} c_n I_{n+1,j}^{(1,z,\pm)} \\
&= \int_0^{C^\pm} \zeta \frac{e^{\pm ikz}e^{\mp kz\zeta^2}}{e^{\pm i\alpha(M+1)d}e^{(M+1)kd(\zeta^2-i)}-e^{\pm i\alpha Md}e^{Mkd(\zeta^2-i)}} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&\quad + e^{\pm ikz}\sum_{j=1}^{M} e^{i(k\mp\alpha)dj}\sum_{n=0}^{\infty} b_{2n} I_{2n+1,j}^{(0,z,\pm)} + e^{\pm ikz}\sum_{j=1}^{M} e^{i(k\mp\alpha)dj}\sum_{n=1}^{\infty} c_{2n+1} I_{2n+2,j}^{(1,z,\pm)}
\end{aligned}$$

where

$$I_{n,j}^{(0,z,\pm)} = \int_0^{C^\pm} \zeta^n \frac{J_0\Big(k\rho(1-i)\zeta\Big)}{e^{k(dj\pm z)\zeta^2}}d\zeta \text{ and } I_{n,j}^{(1,z,\pm)} = \int_0^{C^\pm} \zeta^n \frac{J_1\Big(k\rho(1-i)\zeta\Big)}{e^{k(dj\pm z)\zeta^2}}d\zeta.$$

Again rather than calculating the integrals $I_{n,j}^{(0,z,\pm)}$ and $I_{n,j}^{(1,z,\pm)}$ directly, Hankel's formula [18] will be used as in (33) to approximate them. More precisely:

$$V_{2n+1,j}^{(0,z,\pm)} = \int_0^{\infty} \zeta^{2n+1} \frac{J_0\Big(k\rho(1-i)\zeta\Big)}{e^{k(dj\pm z)\zeta^2}}d\zeta \text{ and } V_{2n,j}^{(1,z,\pm)} = \int_0^{\infty} \zeta^{2n} \frac{J_1\Big(k\rho(1-i)\zeta\Big)}{e^{k(dj\pm z)\zeta^2}}d\zeta$$

are good approximations for $I_{n,j}^{(0,z,\pm)}$ and $I_{n,j}^{(1,z,\pm)}$. For

$$n < \frac{k\rho^2}{8d} - \frac{\log(\epsilon)}{2} + \frac{k\rho}{4d}\sqrt{\rho^2 - \frac{4d\log(\epsilon)}{k}}$$

we have:

$$\left| I_{2n+1,j}^{(0,z,\pm)} - V_{2n+1,j}^{(0,z,\pm)} \right| < \epsilon C^{\pm} \text{ and } \left| I_{2n,j}^{(1,z,\pm)} - V_{2n,j}^{(1,z,\pm)} \right| < \epsilon C^{\pm}.$$

We will use Hankel's formula to evaluate $V_{2n+1,j}^{(0,z,\pm)}$ and $V_{2n+1,j}^{(1,z,\pm)}$

$$V_{2n+1,j}^{(0,z,\pm)} = \frac{\Gamma(n+1)}{2(k(dj \pm z))^{n+1}} {}_1F_1(n+1, 1; \frac{ik\rho^2}{2(dj \pm z)})$$

and

$$V_{2n,j}^{(1,z,\pm)} = \frac{\Gamma(n+2)(k\rho(1-i))}{4(k(dj \pm z))^{n+2}} {}_1F_1(n+2, 2; \frac{ik\rho^2}{2(dj \pm z)}).$$

Finally, as in (38), $G(\rho, z)$ can be expressed in the form:

$$\begin{aligned}
G(\rho, z) \approx \frac{e^{ikr}}{4\pi r} &+ \frac{k}{2\pi}\int_0^{C_{\mathrm{M}}^{+}} \zeta \frac{e^{ikz}e^{-kz\zeta^2}}{e^{i\alpha dj}e^{(M+1)kd(\zeta^2-i)} - e^{i\alpha dj}e^{Mkd(\zeta^2-i)}} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&+ \frac{k}{2\pi}\int_0^{C_{\mathrm{M}}^{-}} \zeta \frac{e^{-ikz}e^{kz\zeta^2}}{e^{-i\alpha dj}e^{(M+1)kd(\zeta^2-i)} - e^{-i\alpha dj}e^{Mkd(\zeta^2-i)}} J_0\Big(k\rho\zeta\sqrt{\zeta^2-2i}\Big)d\zeta \\
&+ \frac{k}{2\pi}\sum_{j=1}^{M} e^{ikjd}e^{ikz+i(k-\alpha)d}\sum_{n=0}^{N} b_{2n}\frac{n!}{2(k(dj+z))^{n+1}} {}_1F_1\Big(n+1, 1; \frac{ik\rho^2}{2(dj+z)}\Big) \\
&+ \frac{k}{2\pi}\sum_{j=1}^{M} e^{ikjd}e^{ikz+i(k-\alpha)d}\sum_{n=1}^{N} c_{2n+1}\frac{(n+1)!(k\rho(1-i))}{4(k(dj+z))^{n+2}} {}_1F_1\Big(n+2, 2; \frac{ik\rho^2}{2(dj+z)}\Big) \\
&+ \frac{k}{2\pi}\sum_{j=1}^{M} e^{ikjd}e^{-ikz+i(k+\alpha)d}\sum_{n=0}^{N} b_{2n}\frac{n!}{2(k(dj-z))^{n+1}} {}_1F_1\Big(n+1, 1; \frac{ik\rho^2}{2(dj-z)}\Big) \\
&+ \frac{k}{2\pi}\sum_{j=1}^{M} e^{ikjd}e^{-ikz+i(k+\alpha)d}\sum_{n=1}^{N} c_{2n+1}\frac{(n+1)!(k\rho(1-i))}{4(k(dj-z))^{n+2}} {}_1F_1\Big(n+2, 2; \frac{ik\rho^2}{2(dj-z)}\Big)
\end{aligned}$$

where the integrals are truncated to $[0, C_{\mathrm{new}}^{\pm}]$ with:

$$C_{\mathrm{M}}^{\pm} = \frac{\rho + \sqrt{\rho^2 - \frac{4(Md\pm z)\log(\epsilon)}{k}}}{2(Md \pm z)}.$$

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