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RAPID EVALUATION OF NONREFLECTING BOUNDARY KERNELS FOR TIME-DOMAIN WAVE PROPAGATION*

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Abstract. We present a systematic approach to the computation of exact nonreflecting boundary conditions for the wave equation. In both two and three dimensions, the critical step in our analysis involves convolution with the inverse Laplace transform of the logarithmic derivative of a Hankel function. The main technical result in this paper is that the logarithmic derivative of the Hankel function $H_\nu^{(1)}(z)$ of real order ν can be approximated in the upper half z-plane with relative error ε by a rational function of degree $d \sim O(\log|\nu| \log\frac{1}{\varepsilon} + \log^2|\nu| + |\nu|^{-1}\log^2\frac{1}{\varepsilon})$ as $|\nu| \to \infty$, $\varepsilon \to 0$, with slightly more complicated bounds for $\nu = 0$. If N is the number of points used in the discretization of a cylindrical (circular) boundary in two dimensions, then, assuming that $\varepsilon < 1/N$, $O(N \log N \log\frac{1}{\varepsilon})$ work is required at each time step. This is comparable to the work required for the Fourier transform on the boundary. In three dimensions, the cost is proportional to $N^2 \log^2 N + N^2 \log N \log\frac{1}{\varepsilon}$ for a spherical boundary with N^2 points, the first term coming from the calculation of a spherical harmonic transform at each time step. In short, nonreflecting boundary conditions can be imposed to any desired accuracy, at a cost dominated by the interior grid work, which scales like N^2 in two dimensions and N^3 in three dimensions.

Key words. Bessel function, approximation, high-order convergence, wave equation, Maxwell's equations, nonreflecting boundary condition, radiation boundary condition, absorbing boundary condition

AMS subject classifications. 33C10, 41A20, 44A10, 44A35, 65D20

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1. Introduction.

A longstanding practical issue in numerical wave propagation and scattering problems concerns the reduction of an unbounded domain to a bounded domain by the imposition of nonreflecting boundary conditions at an artificial boundary. We restrict our attention to "time-domain" calculations, for which it is well-known that the exact nonreflecting conditions are global in both space and time. While the problem has been widely studied (see Givoli [1] for an overview), the boundary conditions used in practice typically introduce serious numerical artifacts. An exception is the method developed by Ting and Miksis [2], which relies on Kirchhoff's formula to solve the wave equation in an exterior domain, but which is computationally expensive. The two most common approaches are based on the construction of local differential boundary conditions [3, 4] or absorbing regions [5, 6], but neither provides a clear sequence of approximations which converge to the exact, nonlocal conditions. Recently, Sofronov [7] and, independently, Grote and Keller [8]

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have developed and implemented an integrodifferential approach for three-dimensional calculations using a spherical boundary and have demonstrated that high accuracy can be achieved at reasonable cost. In their schemes, the work is of the same order as the explicit finite difference or finite element calculation in the interior of the domain. For N^2 points on the spherical boundary, $O\big(N^3\big)$ work is required. Hagstrom and Hariharan [9] have shown that these conditions can be effectively implemented using only local operators, but at the cost of introducing a large number of auxiliary functions at the boundary. A somewhat more general, but closely related, integral formulation is introduced in [10, 11, 12]. The fundamental analytical tool in the latter papers is what we refer to as the *nonreflecting boundary kernel* which is the inverse Laplace transform of the logarithmic derivative of a Hankel function.

In this paper, we prove that the logarithmic derivative of a Hankel function can be approximated as a ratio of polynomials of modest degree, so that its inverse Laplace transform can be expressed as a sum of exponentials. Our analytical approach combines an extension of the Mittag–Leffler theorem with the approximation techniques of the fast multipole method. In particular, Theorem 4.1 presents an exact representation of the logarithmic derivative as a sum of poles plus a continuous density on the branch cut. Theorem 4.6, which is preceded by several technical lemmas, presents a reduced, approximate representation.

Using this approach, the cost of computing the nonreflecting boundary condition is comparable to that of a fast Fourier or spherical harmonic transform. For two-dimensional problems, $O(N \log N \log \frac{1}{\varepsilon})$ work is required at each time step, where N is the number of points used in the discretization of a cylindrical (circular) boundary. In three dimensions, the cost is proportional to $N^2 \log^2 N + N^2 \log N \log \frac{1}{\varepsilon}$ for a spherical boundary with N^2 points. The first term comes from the calculation of the spherical harmonic transform using the fast algorithm of [13, 14].

Other authors, including Nédélec [15] and Cruz and Sesma [16], have studied the logarithmic derivative of the Hankel function, based on a variety of techniques. In this paper we present a sum-of-poles representation for the logarithmic derivative of a Hankel function of real order ν bounded away from zero with accuracy ε for argument, z, satisfying $\mathrm{Im}(z) \geq 0$. The number of poles is bounded by $O\big(\log|\nu| \cdot \log\frac{1}{\varepsilon} + \log^2|\nu| + |\nu|^{-1}\log^2\frac{1}{\varepsilon}\big)$. A similar representation for $\nu = 0$ is also derived which is valid for $\mathrm{Im}(z) \geq \eta > 0$ requiring $O\big(\log\frac{1}{\eta} \cdot \log\frac{1}{\varepsilon} + \log\frac{1}{\varepsilon} \cdot \log\log\frac{1}{\varepsilon} + \log\frac{1}{\eta} \cdot \log\log\frac{1}{\eta}\big)$ poles.

In section 2, we introduce nonreflecting boundary kernels. In section 3 we collect background material in a form convenient for the subsequent development. Section 4 contains the analytical and approximate treatment of the logarithmic derivative, while a procedure for computing these representations is presented in Section 5. The results of our numerical computations are contained in section 6, and we present our conclusions in section 7.

2. Nonreflecting boundary kernels. Let us first consider the wave equation

$$u_{tt} = c^2 \nabla^2 u \tag{2.1}$$

in a two-dimensional annular domain $\rho_0 < \rho < \rho_1$. The general solution can be expressed as

$$u(\rho, \phi, t) = \sum_{n=-\infty}^{\infty} e^{in\phi}\, \mathcal{L}^{-1}\big[a_n(s)\, K_n(\rho s/c) + b_n(s)\, I_n(\rho s/c)\big](t), \tag{2.2}$$

where K_n and I_n are modified Bessel functions (see, for example, [17, section 9.6]),

$$K_n(z) = \frac{\pi}{2} i^{n+1} H_n^{(1)}\big(z\, e^{\pi i/2}\big), \qquad I_n(z) = i^{-n} J_n\big(z\, e^{\pi i/2}\big), \qquad -\pi < \arg z \le \frac{\pi}{2}, \tag{2.3}$$

the coefficients a_n and b_n are arbitrary functions analytic in the right half-plane, $\mathcal{L}$ denotes the Laplace transform

$$\mathcal{L}[f](s) = \int_0^\infty e^{-st} f(t)\, dt, \tag{2.4}$$

and $\mathcal{L}^{-1}$ denotes the inverse Laplace transform

$$\mathcal{L}^{-1}[g](t) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} e^{st} g(s)\, ds. \tag{2.5}$$

Likewise, for the wave equation in a three-dimensional domain $r_0 < r < r_1$, the general solution can be expressed as

$$u(r,\phi,\theta,t) = \sum_{n=-\infty}^{\infty} \sum_{m=-n}^{n} Y_{nm}(\phi,\theta)\, \mathcal{L}^{-1}\left[a_{nm}(s)\, \frac{K_{n+\frac{1}{2}}(rs/c)}{\sqrt{rs/c}} + b_{nm}(s)\, \frac{I_{n+\frac{1}{2}}(rs/c)}{\sqrt{rs/c}} \right](t). \tag{2.6}$$

If we imagine that $\rho = \rho_1$ (or $r = r_1$) is to be used as a nonreflecting boundary, then we can assume there are no sources in the exterior region and the coefficients $b_n(s)$ (or $b_{nm}(s)$) are zero. Let us now denote by $u_n(\rho,t)$ the function satisfying

$$\mathcal{L}[u_n](\rho,s) = a_n(s)\, K_n(\rho s/c). \tag{2.7}$$

Then

$$\begin{aligned} \mathcal{L}\Big[\frac{\partial}{\partial\rho} u_n\Big](\rho,s) &= a_n(s) \cdot \frac{s}{c} \cdot K_n'(\rho s/c) \\ &= \mathcal{L}[u_n](\rho,s) \cdot \Big(\frac{s}{c}\, \frac{K_n'(\rho s/c)}{K_n(\rho s/c)}\Big), \end{aligned} \tag{2.8}$$

so that

$$\frac{\partial}{\partial\rho} u_n(\rho,t) = u_n(\rho,t) * \mathcal{L}^{-1}\left[\frac{s}{c}\, \frac{K_n'(\rho s/c)}{K_n(\rho s/c)} \right](t), \tag{2.9}$$

where $*$ denotes Laplace convolution

$$(f * g)(t) = \int_0^t f(\tau)\, g(t-\tau)\, d\tau. \tag{2.10}$$

The convolution kernel in (2.9) is a generalized function. Its singular part is easily removed, however, by subtracting the first two terms of the asymptotic expansion

$$\frac{s}{c}\, \frac{K_n'(\rho s/c)}{K_n(\rho s/c)} \sim -\frac{s}{c} - \frac{1}{2\rho} + O\big(s^{-1}\big), \qquad s \to \infty. \tag{2.11}$$

From the assumption $u_n(\rho,t)=0$ for $t\le 0$ and standard properties of the Laplace transform we obtain the boundary condition

$$\frac{\partial}{\partial\rho}u_n(\rho,t)+\frac{1}{c}\frac{\partial}{\partial t}u_n(\rho,t)+\frac{1}{2\rho}u_n(\rho,t)=\int_0^t \sigma_n(t-\tau)\,u_n(\rho,\tau)\,d\tau, \tag{2.12}$$

where

$$\sigma_n(t)=\mathcal{L}^{-1}\left[\frac{s}{c}+\frac{1}{2\rho}+\frac{s}{c}\frac{K_n'(\rho s/c)}{K_n(\rho s/c)}\right](t), \tag{2.13}$$

which we impose at $\rho=\rho_1$.

Remark. The solution to the wave equation in physical space is recovered on the nonreflecting boundary from u_n by Fourier transformation:

$$u(\rho_1,\phi,t)=\sum_{n=-N/2}^{N/2-1} u_n(\rho_1,t)\,e^{in\phi}, \tag{2.14}$$

assuming N points are used in the discretization.

The analogous boundary condition in three dimensions is expressed in terms of the functions $u_{nm}(r,t)$ satisfying

$$\mathcal{L}[u_{nm}](r,s)=a_{nm}(s)\,\frac{K_{n+\frac{1}{2}}(rs/c)}{\sqrt{rs/c}}. \tag{2.15}$$

After some algebraic manipulation, assuming $u_{nm}(r,t)=0$ for $t\le 0$, we have

$$\frac{\partial}{\partial r}u_{nm}(r,t)+\frac{1}{c}\frac{\partial}{\partial t}u_{nm}(r,t)+\frac{1}{r}u_{nm}(r,t)=\int_0^t \omega_n(t-\tau)\,u_{nm}(r,\tau)\,d\tau, \tag{2.16}$$

where

$$\omega_n(t)=\mathcal{L}^{-1}\left[\frac{s}{c}+\frac{1}{2r}+\frac{s}{c}\frac{K_{n+\frac{1}{2}}'(rs/c)}{K_{n+\frac{1}{2}}(rs/c)}\right](t), \tag{2.17}$$

which we impose at $r=r_1$.

Note that the boundary conditions (2.12) and (2.16) are exact but nonlocal, since they rely on a Fourier (or spherical harmonic) transformation in space and are history dependent. The form of the history is simple, however, and expressed, for each separate mode, in terms of a convolution kernel which is the inverse Laplace transform of a function defined in terms of the logarithmic derivative of a modified Bessel function

$$\frac{d}{dz}\log K_\nu(z)=\frac{K_\nu'(z)}{K_\nu(z)}. \tag{2.18}$$

Remark. In three dimensions, the required logarithmic derivative of $K_{n+\frac{1}{2}}(z)$ is a ratio of polynomials, so that one can recast the boundary condition in terms of a differential operator of order n. The resulting expression would be equivalent to those derived by Sofronov [7] and Grote and Keller [8].

The remainder of this paper is devoted to the approximation of the logarithmic derivatives (2.18) as a ratio of polynomials of degree $O(\log\nu)$, from which the convolution kernels σ_n and ω_n can be expressed as a sum of decaying exponentials. This

representation allows for the recursive evaluation of the integral operators in (2.12) and (2.16), using only $O(\log n)$ work per time step (see [18]). We note that, by Parseval's equality, the L_2 error resulting from convolution with an approximate kernel is sharply bounded by the L_∞ error in the approximation to the kernel's transform. Precisely, approximating the kernel $B(t)$ by the kernel $A(t)$ we find

$$\begin{aligned}\big\|A*u-B*u\big\|_2=\big\|\hat{A}\hat{u}-\hat{B}\hat{u}\big\|_2 &\le \sup_{s\in i\mathbb{R}}\frac{\big|\hat{A}-\hat{B}\big|}{\big|\hat{B}\big|}\big\|\hat{B}\hat{u}\big\|_2\\ &= \sup_{s\in i\mathbb{R}}\frac{\big|\hat{A}-\hat{B}\big|}{\big|\hat{B}\big|}\big\|B*u\big\|_2,\end{aligned}\tag{2.19}$$

where we assume that $\hat{A}$, $\hat{B}$, and $\hat{u}$ are all regular for $\mathrm{Re}(s)>0$. For finite times we may let s have a positive real part, η:

$$\big\|A*u-B*u\big\|_{L_2(0,T)}\le e^{\eta T}\sup_{s\in\eta+i\mathbb{R}}\frac{\big|\hat{A}-\hat{B}\big|}{\big|\hat{B}\big|}\big\|B*u\big\|_{L_2(0,T)}.\tag{2.20}$$

We therefore concentrate our theoretical developments on L_∞ approximations. For ease of computation, however, we compute our rational representations by least squares methods. These do generally lead to small relative errors in the maximum norm, as will be shown.

Since Hankel functions are more commonly used in the special function literature, we will write the logarithmic derivatives as

$$\frac{d}{dz}\log K_\nu(z)=\frac{d}{dz}\log H_\nu^{(1)}\big(z\,e^{\pi i/2}\big)=i\,\frac{H_\nu^{(1)'}\big(z\,e^{\pi i/2}\big)}{H_\nu^{(1)}\big(z\,e^{\pi i/2}\big)}.\tag{2.21}$$

We are, then, interested in approximating logarithmic derivative of the Hankel function on and above the real axis.

3. Mathematical preliminaries. In this section we collect several well-known facts concerning the Bessel equation, the logarithmic derivative of the Hankel function, and pole expansions, in a form that will be useful in the subsequent analytical development.

3.1. Bessel's equation. Bessel's differential equation

$$\frac{d^2u}{dz^2}+\frac{1}{z}\frac{du}{dz}+\Big(1-\frac{\nu^2}{z^2}\Big)u=0,\tag{3.1}$$

for $\nu\in\mathbb{R}$, has linearly independent solutions $H_\nu^{(1)}$ and $H_\nu^{(2)}$, known as Hankel's functions. These can be expressed by the formulae

$$H_\nu^{(1)}(z)=\frac{J_{-\nu}(z)-e^{-\nu\pi i}J_\nu(z)}{i\sin(\nu\pi)},\qquad H_\nu^{(2)}(z)=-\frac{J_{-\nu}(z)-e^{\nu\pi i}J_\nu(z)}{i\sin(\nu\pi)},\tag{3.2}$$

where the Bessel function of the first kind is defined by

$$J_\nu(z)=\big(\frac{z}{2}\big)^\nu\sum_{k=0}^{\infty}\frac{(-z^2/4)^k}{k!\Gamma(\nu+k+1)}.\tag{3.3}$$

The expressions in (3.2) are replaced by their limiting values for integer values of ν. (See, for example, [17, section 9.1].) For general ν, the functions $H_\nu^{(1)}$ and $H_\nu^{(2)}$ have a branch point at $z = 0$ and it is customary to place the corresponding branch cut on the negative real axis and impose the restriction $-\pi < \arg z \le \pi$. We shall find it more convenient, however, to place the branch cut on the negative imaginary axis, with the restriction

$$-\frac{\pi}{2} \le \arg z < \frac{3\pi}{2}. \tag{3.4}$$

Hankel's functions have especially simple asymptotic properties. In particular (see, for example, [19, section 7.4.1]),

$$H_\nu^{(1)}(z) \sim \Big(\frac{2}{\pi z}\Big)^{1/2} e^{i(z-\nu\pi/2-\pi/4)} \sum_{k=0}^{\infty} i^k \, \frac{A_k(\nu)}{z^k}, \tag{3.5}$$

$$H_\nu^{(1)'}(z) \sim \Big(\frac{2}{\pi z}\Big)^{1/2} e^{i(z-\nu\pi/2-\pi/4)} \sum_{k=0}^{\infty} i^k \, \frac{A_k(\nu)}{z^k}\Big(-\frac{1}{2z} + i - \frac{k}{z}\Big) \tag{3.6}$$

as $z \to \infty$, with $-\pi + \delta \le \arg z \le 2\pi - \delta$, where

$$A_k(\nu) = \frac{(4\nu^2 - 1^2)(4\nu^2 - 3^2)\cdots(4\nu^2 - (2k-1)^2)}{k!\, 8^k}, \tag{3.7}$$

and the branch of the square root is determined by

$$z^{1/2} = e^{(\log|z| + i\arg z)/2}. \tag{3.8}$$

Finally we note the symmetry

$$H_\nu^{(1)}(z) = e^{-\nu\pi i} H_{-\nu}^{(1)}(z). \tag{3.9}$$

We also make use of the modified Bessel functions $K_\nu(z)$ and $I_\nu(z)$. These are linearly independent solutions of the equation obtained from (3.1) by the transformation $z \to iz$. Their Wronskian satisfies

$$K_\nu(z) I_\nu'(z) - K_\nu'(z) I_\nu(z) = z^{-1}. \tag{3.10}$$

Moreover we have for positive r [20]

$$H_\nu^{(1)}(re^{-i\pi/2}) = \frac{2}{\pi i} e^{-\nu\pi i/2}\big(e^{\nu\pi i} K_\nu(r) + \pi i I_\nu(r)\big). \tag{3.11}$$

Asymptotic expansions of $K_\nu(r)$ and $I_\nu(r)$ for r small and large are also known [17, sections 9.6 and 9.7]. For real r and $\nu \ge 0$ we have

$$K_\nu(r) \sim \begin{cases} \gamma - \log\dfrac{r}{2}, & \nu = 0, \\ \dfrac{\Gamma(\nu)}{2}\Big(\dfrac{r}{2}\Big)^{-\nu}, & \nu > 0, \end{cases} \qquad r \to 0, \tag{3.12}$$

$$I_\nu(r) \sim \frac{1}{\Gamma(\nu+1)}\Big(\frac{r}{2}\Big)^{\nu}, \qquad r \to 0, \tag{3.13}$$

$$K_\nu(r) \sim \sqrt{\frac{\pi}{2r}}\, e^{-r}, \qquad r \to \infty, \tag{3.14}$$

$$I_\nu(r) \sim \sqrt{\frac{1}{2\pi r}}\, e^{r}, \qquad r \to \infty. \tag{3.15}$$

Here $\gamma = 0.5772\ldots$ is the Euler constant.

Finally, we note the uniform expansions of Bessel functions for $\nu \to \infty$ given in [17]. For Hankel function and derivative we have

$$H_\nu^{(1)}(\nu z) \sim 2e^{-\pi i/3}\Big(\frac{4\zeta}{1-z^2}\Big)^{1/4}\frac{\mathrm{Ai}\big(e^{2\pi i/3}\nu^{2/3}\zeta\big)}{\nu^{1/3}}, \tag{3.16}$$

$$H_\nu^{(1)'}(\nu z) \sim \frac{4e^{-2\pi i/3}}{z}\Big(\frac{4\zeta}{1-z^2}\Big)^{-1/4}\frac{\mathrm{Ai}'\big(e^{2\pi i/3}\nu^{2/3}\zeta\big)}{\nu^{2/3}} \tag{3.17}$$

as $\nu \to \infty$, where we restrict z to $|\arg(z)| \le \pi/2$ and define

$$\frac{2}{3}\zeta^{3/2} = \log\frac{1+\sqrt{1-z^2}}{z} - \sqrt{1-z^2}. \tag{3.18}$$

Here, $\mathrm{Ai}(t)$ denotes the Airy function [17, section 10.4]. Note that $\zeta = 0$ when $z = 1$. Large ν approximations of the modified Bessel functions for real arguments, r, are given by

$$K_\nu(\nu r) \sim \sqrt{\frac{\pi}{2\nu}}\,\frac{e^{-\nu\,\phi(r)}}{\big(1+r^2\big)^{1/4}}, \qquad I_\nu(\nu r) \sim \frac{1}{\sqrt{2\pi\nu}}\,\frac{e^{\nu\,\phi(r)}}{\big(1+r^2\big)^{1/4}}, \qquad \nu \to \infty, \tag{3.19}$$

where

$$\phi(r) = \log\frac{r}{1+\sqrt{1+r^2}} + \sqrt{1+r^2}. \tag{3.20}$$

3.2. Hankel function logarithmic derivative. We denote the logarithmic derivative of $H_\nu^{(1)}$ by G_ν,

$$G_\nu(z) = \frac{d}{dz}\log H_\nu^{(1)}(z) = \frac{H_\nu^{(1)'}(z)}{H_\nu^{(1)}(z)}. \tag{3.21}$$

The following lemma states a few fundamental facts about G_ν that we will use below.

LEMMA 3.1. *The function $G_\nu(z)$, for $\nu \in \mathbb{R}$, satisfies the formulae*

$$G_{-\nu}(z) = G_\nu(z), \tag{3.22}$$

$$G_\nu(\overline{z}\,e^{\pi i}) = \overline{G_\nu(z)}\,e^{\pi i}, \qquad -\frac{\pi}{2} < \arg z \le \frac{\pi}{2}, \tag{3.23}$$

where $\overline{z} = |z|\,e^{-i\arg z}$ is the complex conjugate of z. Asymptotic approximations to G_ν are

$$G_\nu(z) \sim \begin{cases} \big(\log(z\,e^{-\pi i/2}/2)+\gamma\big)^{-1}\,z^{-1} + O(z), & \nu = 0, \\ -|\nu|\,z^{-1} + O(z^{2|\nu|-1}), & 0 < |\nu| < 1, \\ -|\nu|\,z^{-1} + O(z\log z), & |\nu| = 1, \\ -|\nu|\,z^{-1} + O(z), & |\nu| > 1, \end{cases} \qquad z \to 0, \tag{3.24}$$

where γ is the Euler constant,

$$G_\nu(z) \sim \sum_{k=0}^{\infty} i^k\frac{A_k(\nu)}{z^k}\Big(-\frac{1}{2z}+i-\frac{k}{z}\Big)\Big/\sum_{k=0}^{\infty} i^k\frac{A_k(\nu)}{z^k}, \qquad z \to \infty, \tag{3.25}$$

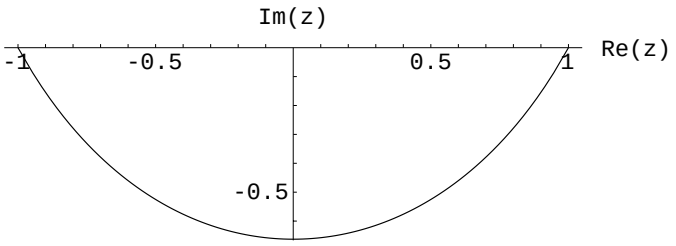

FIG. 3.1. *Curve $z(\zeta)$ defined by* (3.18) *near which the scaled zeros of $H_\nu^{(1)}$ lie (see Lemma* 3.2*). The branch cut of $H_\nu^{(1)}$ is chosen* (3.4) *on the negative imaginary axis.*

where $A_k(\nu)$ is defined in (3.7)*, and*

$$G_\nu(\nu z) \sim \frac{2e^{-\pi i/3}}{\nu^{1/3} z}\Big(\frac{4\zeta}{1-z^2}\Big)^{-1/2} \frac{\mathrm{Ai}'\big(e^{2\pi i/3}\nu^{2/3}\zeta\big)}{\mathrm{Ai}\big(e^{2\pi i/3}\nu^{2/3}\zeta\big)}, \qquad \nu \to \infty, \tag{3.26}$$

where ζ is defined in (3.18)*. Furthermore, the function u_ν defined by*

$$u_\nu(z) = z\, G_\nu(z) \tag{3.27}$$

satisfies the recurrence

$$u_\nu(z) = \frac{z^2}{\nu - 1 - u_{\nu-1}(z)} - \nu. \tag{3.28}$$

Proof. Equations (3.22) and (3.23) and asymptotic expansion (3.24) follow immediately from the definitions (3.2) through (3.4) of J_ν and $H_\nu^{(1)}$. The asymptotic expansion (3.25) follows from (3.5) and (3.6), while (3.26) is a consequence of (3.16) and (3.17). The recurrence (3.28) from standard Bessel recurrences [17, section 9.1.27]. ∎

The zeros of $H_\nu^{(1)}(z)$ are well characterized [17, 20]; they lie in the lower half z-plane near the curve shown in Figure 3.1, obtained by transformation [21] of Bessel's equation. In terms of the asymptotic approximation (3.16), this curve corresponds to negative, real arguments of the Airy function.

LEMMA 3.2. *The zeros $h_{\nu,1}, h_{\nu,2}, \ldots$ of $H_\nu^{(1)}(z)$ in the sector $-\pi/2 \le \arg z \le 0$ are given by the asymptotic expansion*

$$h_{\nu,n} \sim \nu\, z(\zeta_n) + O\big(\nu^{-1}\big), \qquad \begin{array}{l}\nu \to \infty,\\ n = 1, \ldots, \lfloor |\nu|/2 + 1/4 \rfloor,\end{array} \tag{3.29}$$

uniformly in n, where ζ_n is defined by the equation

$$\zeta_n = e^{-2\pi i/3}\nu^{-2/3} a_n, \tag{3.30}$$

$z(\zeta)$ is obtained from inverting (3.18)*, and a_n is the nth negative zero of Airy function* Ai*. The zeros in the sector $\pi \le \arg z \le 3\pi/2$ are given by $-\overline{h_{\nu,1}}, -\overline{h_{\nu,2}}, \ldots$. In particular,*

$$h_{\nu,1} \sim \nu + e^{-2\pi i/3}(\nu/2)^{1/3}(-a_1), \tag{3.31}$$

where $-a_1 = 2.338\ldots$.

3.3. Pole expansions. A set of poles in a finite region defines a function that is smooth away from the region, with the smoothness increasing as the distance increases. This fact leads to the following approximation related to the fast multipole method [22, 23].

LEMMA 3.3. *Suppose that $q_1, \ldots, q_n$ are complex numbers and $z_1, \ldots, z_n$ are complex numbers with $|z_j| \le 1$ for $j = 1, \ldots, n$. The function*

$$f(z) = \sum_{j=1}^{n} \frac{q_j}{z - z_j} \tag{3.32}$$

can be approximated for $\mathrm{Re}(z) = a > 1$ *by the m pole expansion*

$$g_m(z) = \sum_{j=0}^{m-1} \frac{\gamma_j}{z - \omega^j}, \tag{3.33}$$

where $\omega = e^{2\pi i/m}$ is a root of unity and γ_j is defined by

$$\gamma_j = \frac{1}{m} \sum_{l=0}^{m-1} \omega^{-jl} \sum_{k=1}^{n} q_k \, {z_k}^l, \qquad j = 0, \ldots, m-1. \tag{3.34}$$

The error of the approximation is bounded by

$$\big|f(z) - g_m(z)\big| \le \frac{2(a^2+1)}{(a^m-1)(a-1)^2} |F(z)|, \tag{3.35}$$

where

$$F(z) = \sum_{j=1}^{n} \frac{|q_j|}{z - z_j}. \tag{3.36}$$

Proof. We use the geometric series summation

$$\frac{1}{z-v} = \sum_{k=0}^{m-1} \frac{v^k}{z^{k+1}} + \frac{v^m}{z^m} \frac{1}{z-v} \tag{3.37}$$

to obtain

$$\begin{aligned} f(z) - g_m(z) = {} & \sum_{k=0}^{m-1} \frac{1}{z^{k+1}} \Big(\sum_{j=1}^{n} q_j \, {z_j}^k - \sum_{j=0}^{m-1} \gamma_j \, \omega^{jk} \Big) \\ & + \frac{1}{z^m} \Big(\sum_{j=1}^{n} \frac{q_j \, {z_j}^m}{z - z_j} - \sum_{j=0}^{m-1} \frac{\gamma_j \, \omega^{jm}}{z - \omega^j} \Big). \end{aligned} \tag{3.38}$$

All m terms of the first summation vanish, due to the combination of (3.34) and the equality $\sum_{j=0}^{m-1} \omega^{jk} = m\,\delta_{k0}$. For the error term we obtain

$$\begin{aligned}\left|\sum_{j=1}^{n}\frac{q_j\,{z_j}^m}{z-z_j}\right| &\le \sum_{j=1}^{n}\left|\frac{q_j\,{z_j}^m}{z-z_j}\right| \le \frac{1}{|z|}\sum_{j=1}^{n}\frac{|q_j|}{\left|1-z_j/z\right|}\\ &\le \frac{1}{|z|}\,\frac{a^2+1}{(a-1)^2}\sum_{j=1}^{n}\frac{(1-a^{-1})|q_j|}{1+a^{-2}} \le \frac{a^2+1}{(a-1)^2}\,\frac{1}{|z|}\,\mathrm{Re}\left(\sum_{j=1}^{n}\frac{|q_j|}{1-z_j/z}\right)\\ &\le \frac{a^2+1}{(a-1)^2}\left|\sum_{j=1}^{n}\frac{|q_j|}{z-z_j}\right| = \frac{a^2+1}{(a-1)^2}\,|F(z)|, \qquad (3.39)\end{aligned}$$

and

$$\left|\sum_{j=0}^{m-1}\frac{\gamma_j\,\omega^{jm}}{z-\omega^j}\right| = \left|\sum_{j=0}^{m-1}\frac{\gamma_j}{z-\omega^j}\right| = \big|g_m(z)\big|. \qquad (3.40)$$

Moreover, repeating the computations of (3.39), we find

$$|f(z)| \le \frac{a^2+1}{(a-1)^2}|F(z)|. \qquad (3.41)$$

Now the combination of (3.38) through (3.41) and the triangle inequality gives (3.35). □

Inequality (3.35) remains valid if we assume instead that $|z_j| \le b$ and $\mathrm{Re}(z) = ab > b$, for arbitrary $b \in \mathbb{R}$, $b > 0$; this fact leads to the next two results whose proofs mimic that of Lemma 3.3 and are omitted.

LEMMA 3.4. *Suppose n, p are positive integers, $q_1, \ldots, q_n$ are complex numbers, and $z_1, \ldots, z_n$ are complex numbers contained in disks $D_1, \ldots, D_p$ of radii $r_1, \ldots, r_p$, centered at $c_1, \ldots, c_p$, respectively. The function*

$$f(z) = \sum_{j=1}^{n}\frac{q_j}{z-z_j} \qquad (3.42)$$

can be approximated for z satisfying $\mathrm{Re}(z-c_i) \ge a r_i > r_i$ for $i = 1, \ldots, p$ by the $m \cdot p$ pole expansion

$$g_m(z) = \sum_{i=1}^{p}\sum_{j=0}^{m-1}\frac{\gamma_{ij}}{z-(c_i + r_i\,\omega^j)}, \qquad (3.43)$$

where γ_{ij} is defined by

$$\gamma_{ij} = \frac{1}{m}\sum_{l=0}^{m-1}\omega^{-jl}\sum_{z_k \in D_i \setminus U_{i-1}} q_k \cdot \Big(\frac{z_k - c_i}{r_i}\Big)^l, \qquad \begin{matrix} i = 1, \ldots, p, \\ j = 0, \ldots, m-1, \end{matrix} \qquad (3.44)$$

with $U_i = \cup_{j \le i} D_j$. The error of the approximation is bounded by

$$\big|f(z) - g_m(z)\big| \le \frac{2(a^2+1)\,|F(z)|}{(a^m-1)(a-1)^2}, \qquad (3.45)$$

where

$$F(z) = \sum_{j=1}^{n} \frac{|q_j|}{z - z_j}. \tag{3.46}$$

LEMMA 3.5. *Suppose that the discrete poles of Lemma* 3.4 *are replaced with a density q defined on a curve C with $C \subset U_p = D_1 \cup \cdots \cup D_p$, specifically*

$$f(z) = \int_C \frac{q(\zeta)}{z - \zeta}\, d\zeta, \tag{3.47}$$

which is finite for z outside U_p, and that g_m is defined by (3.43) *with γ_{ij} defined by*

$$\gamma_{ij} = \frac{1}{m} \sum_{l=0}^{m-1} \omega^{-jl} \int_{C \cap (D_i \setminus U_{i-1})} q(\zeta) \Big(\frac{\zeta - c_i}{r_i} \Big)^l \, d\zeta, \qquad \begin{matrix} i = 1, \ldots, p, \\ j = 0, \ldots, m-1, \end{matrix} \tag{3.48}$$

with $U_i = \cup_{j \le i} D_j$. Then the bound (3.45) *holds as before.* Lemma 3.3 enables us to approximate, with exponential convergence, a function defined as a sum of poles. The fundamental assumption is that the region of interest be "separated" from the pole locations. The notion of separation is effectively relaxed by covering the pole locations with disks of varying size in an adaptive manner. In Lemmas 3.4 and 3.5, we use this approach to derive our principal analytical result.

4. Rational approximation of the logarithmic derivative. The Hankel function's logarithmic derivative $G_\nu(z)$ defined in (3.21) approaches a constant as $z \to \infty$ and is regular for finite $z \in \mathbb{C}$, except at $z = 0$, which is a branch point, and at the zeros of $H_\nu^{(1)}(z)$, all of which are simple. We can therefore develop a representation for G_ν analogous to that of the Mittag–Leffler theorem; the only addition is due to the branch cut on the negative imaginary axis. It will be convenient to work with $u_\nu(z)$, defined in (3.27), for which approximations to be introduced have simple error bounds.

THEOREM 4.1. *The function $u_\nu(z) = z\, G_\nu(z)$, where G_ν is defined for $\nu \in \mathbb{R}$ by* (3.21) *with the branch cut defined by* (3.4)*, is given by the formula*

$$u_\nu(z) = iz - \frac{1}{2} + \sum_{n=1}^{N_\nu} \frac{h_{\nu,n}}{z - h_{\nu,n}} - \frac{1}{\pi i} \int_0^\infty \frac{\operatorname{Im}\big(u_\nu(re^{-\pi i/2})\big)}{ir + z}\, dr \tag{4.1}$$

for $z \in \mathbb{C}$ not in $\{0, h_{\nu,1}, h_{\nu,2}, \ldots, h_{\nu,N_\nu}\}$ and not on the negative imaginary axis. Here $h_{\nu,1}, h_{\nu,2}, \ldots, h_{\nu,N_\nu}$ denote the zeros of $H_\nu^{(1)}(z)$, which number N_ν.

Proof. The case of the spherical Hankel function, where $\nu = k + 1/2$ for $k \in \mathbb{Z}$, is simple and we consider it first. Here $u_\nu(z)$ is a ratio of polynomials in iz with real coefficients, which is clear from the observation that $u_{1/2}(z) = iz - 1/2$ in combination with the recurrence (3.28). Hence

$$u_\nu(z) = p(z) + \sum_{n=1}^{N_\nu} \frac{\alpha_{\nu,n}}{z - h_{\nu,n}}, \tag{4.2}$$

where p is a polynomial and $\alpha_{\nu,n}$ is the residue of u_ν at $h_{\nu,n}$,

$$\alpha_{\nu,n} = \lim_{z \to h_{\nu,n}} (z - h_{\nu,n})\, u_\nu(z) = h_{\nu,n} \tag{4.3}$$

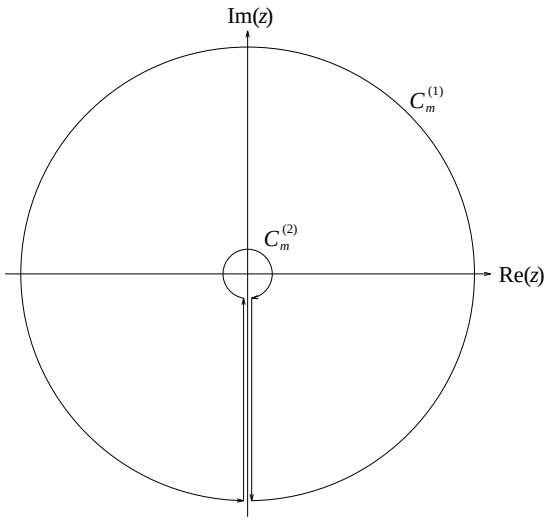

FIG. 4.1. *Integration contour C_m, with inner circle radius $1/m$ and outer radius $m+1$.*

by l'Hôpital's rule. We see from (3.25) that

$$u_\nu(z) \sim iz - \frac{1}{2} + O(z^{-1}), \qquad z \to \infty, \tag{4.4}$$

whence

$$p(z) = iz - \frac{1}{2}. \tag{4.5}$$

Noting that $u_\nu(iy) \in \mathbb{R}$ for $y \in \mathbb{R}$, and combining (4.2), (4.3), and (4.5), we obtain (4.1).

We now consider the case $\nu \neq k+1/2$, $k \in \mathbb{Z}$, for which the origin is a branch point. For $m = 1, 2, \ldots$, we define C_m to be the simple closed curve, shown in Figure 4.1, which proceeds counterclockwise along the circle $C_m^{(1)}$ of radius $m+1$ centered at the origin from $\arg z = -\pi/2$ to $3\pi/2$, to the vertical segment $z = re^{3\pi i/2}$, $r \in [1/m, m+1]$, to the circle $C_m^{(2)}$ of radius $1/m$ centered at the origin from $\arg z = 3\pi/2$ to $-\pi/2$, to the vertical segment $z = re^{-\pi i/2}$, back to the first circle. Since none of the zeros of $H_\nu^{(1)}$ lies on the imaginary axis, C_m encloses them all if m is sufficiently large. For such m, and $z \in \mathbb{C}$ inside C_m with $H_\nu^{(1)}(z) \neq 0$, the residue theorem gives

$$\frac{1}{2\pi i} \int_{C_m} \frac{u_\nu(\zeta)}{\zeta - z}\, d\zeta = u_\nu(z) + \sum_{n=1}^{N_\nu} \frac{h_{\nu,n}}{h_{\nu,n} - z}. \tag{4.6}$$

We now consider the separate pieces of the contour C_m. For the circles $C_m^{(1)}$ and $C_m^{(2)}$, we use the asymptotic expansion (4.4) about infinity and (3.24) about the origin to obtain

$$\lim_{m\to\infty} \frac{1}{2\pi i} \int_{C_m^{(1)}} \frac{u_\nu(\zeta)}{\zeta - z}\, d\zeta = iz - \frac{1}{2}, \qquad \lim_{m\to\infty} \frac{1}{2\pi i} \int_{C_m^{(2)}} \frac{u_\nu(\zeta)}{\zeta - z}\, d\zeta = 0. \tag{4.7}$$

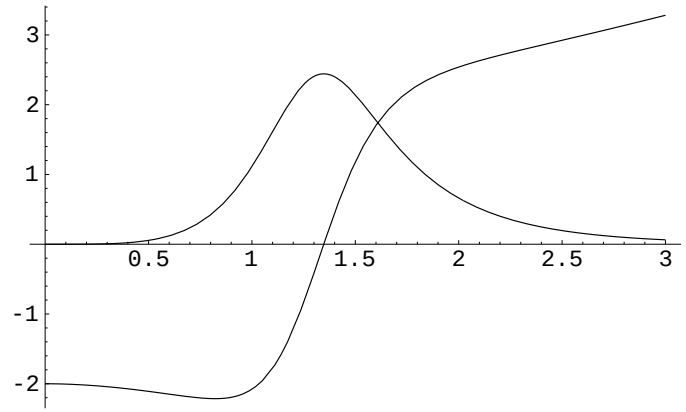

FIG. 4.2. *Plot of* $\mathrm{Re}\big(u_\nu(re^{-\pi i/2})\big)$, *containing the zero crossing, and* $\mathrm{Im}\big(u_\nu(re^{-\pi i/2})\big)$, *for* $\nu = 2$ *and* $r \in [0,3]$.

Now exploiting the symmetry $u_\nu(re^{3\pi i/2}) = \overline{u_\nu(re^{-\pi i/2})}$ from (3.23) for the vertical segments, we obtain

$$\lim_{m\to\infty} \frac{1}{2\pi i}\int_{C_m} \frac{u_\nu(\zeta)}{\zeta - z}\,d\zeta = iz - \frac{1}{2} + \frac{1}{2\pi i}\int_0^\infty \frac{2i\,\mathrm{Im}\big(u_\nu(re^{-\pi i/2})\big)}{(re^{-\pi i/2} - z)}\,e^{-\pi i/2}\,dr, \tag{4.8}$$

which, when combined with (4.6), yields (4.1) and the theorem. □

The primary aim of this paper is to reduce the summation and integral of (4.1) to a similar summation involving dramatically fewer terms. To do so, we restrict z to the upper half-plane and settle for an approximation. Such a representation is possible, for the poles of u_ν (zeros of $H_\nu^{(1)}$) lie entirely in the lower half-plane and do not cluster near the real axis. We first examine the behavior of u_ν on the negative imaginary axis.

The qualitative behavior of u_ν on the branch cut is illustrated by the case of $\nu = 2$, shown in Figure 4.2. The plot changes little with changing ν, except for the sign of $\mathrm{Im}\big(u_\nu(z)\big)$ and the sharpness of its extremum.

LEMMA 4.2. *For* $\nu \in \mathbb{R}$, $\nu \neq k + 1/2$, $k \in \mathbb{Z}$, *the function* $u_\nu(re^{-\pi i/2})$ *is infinitely differentiable on* $r \in (0,\infty)$ *and has imaginary part satisfying the following formulae:*

$$\mathrm{Im}\big(u_\nu(re^{-\pi i/2})\big) = \frac{\pi\cos(\nu\pi)}{\cos^2(\nu\pi)K_\nu^2(r) + \big(\pi I_\nu(r) + \sin(\nu\pi)K_\nu(r)\big)^2} \neq 0, \tag{4.9}$$

$$\mathrm{Im}\big(u_\nu(re^{-\pi i/2})\big) \sim \begin{cases} \dfrac{\pi}{(\log(r/2)+\gamma)^2 + \pi^2}, & \nu = 0, \\ \dfrac{\pi\cos(\nu\pi)}{4^{|\nu|-1}\Gamma(|\nu|)^2}\,r^{2|\nu|}, & \nu \neq 0, \end{cases} \qquad r \to 0, \tag{4.10}$$

$$\mathrm{Im}\big(u_\nu(re^{-\pi i/2})\big) \sim 2\cos(\nu\pi)\,re^{-2r}, \qquad r \to \infty, \tag{4.11}$$

$$\mathrm{Im}\big(u_\nu(re^{-\pi i/2})\big) \sim \frac{\cos(\nu\pi)\sqrt{r^2+\nu^2}}{\cosh\left(2\nu\,\phi(r/|\nu|)\right) + \sin(|\nu|\pi)}, \qquad |\nu| \to \infty, \tag{4.12}$$

where ϕ *is defined in* (3.20).

Proof. Infinite differentiability of $u_\nu(z)$ follows from the observation that $H_\nu^{(1)}(z) \neq 0$ on the negative imaginary axis. To derive (4.9) we recall (3.11) to obtain

$$\mathrm{Im}\big(u_\nu(re^{-\pi i/2})\big) = \frac{r\pi\cos(\nu\pi)\big(K_\nu(r)I'_\nu(r) - K'_\nu(r)I_\nu(r)\big)}{\cos^2(\nu\pi)K_\nu^2(r) + \big(\pi I_\nu(r) + \sin(\nu\pi)K_\nu(r)\big)^2}, \tag{4.13}$$

then apply (3.10). The remaining formulas follow from the asymptotic forms of $K_\nu(r)$ and $I_\nu(r)$ for small and large r, and the uniform large ν expansions given in (3.12) through (3.15) and (3.19). Here we use the symmetry $u_{-\nu} = u_\nu$. Note that (4.10) is valid for $r/|\nu| \to 0$. The approximation (4.12) is nonuniform for $\nu \approx 2k - 1/2$ and $\pi I_\nu(r) + \sin(\nu\pi)K_\nu(r) \approx 0$. ∎

LEMMA 4.3. *Given $\nu_0 > 0$ there exist constants c_0 and c_1 such that for all $\nu \in \mathbb{R}$, $|\nu| \geq \nu_0$, $\nu \neq k + 1/2$, $k \in \mathbb{Z}$, and all z satisfying $\mathrm{Im}(z) \geq 0$, the function*

$$f(z) = \int_0^\infty \frac{\mathrm{Im}\big(u_\nu(re^{-\pi i/2})\big)}{ir + z}\, dr \tag{4.14}$$

satisfies the bounds

$$\frac{c_0}{1 + |z|/|\nu|} \leq |f(z)| \leq \frac{c_1}{1 + |z|/|\nu|}. \tag{4.15}$$

Moreover, there exists $\delta > 0$ such that for all $\nu \in \mathbb{R}$, $|\nu| \geq \nu_0$, and ε with $0 < \varepsilon < 1/2$, $f(z)$ admits an approximation $g(z)$ that is a sum of $d \leq \delta \cdot \big(1 + |\nu|^{-1}\log(1/\varepsilon)\big) \cdot \log(1/\varepsilon)$ poles, with

$$|f(z) - g(z)| \leq \varepsilon \cdot |f(z)|, \tag{4.16}$$

provided $\mathrm{Im}(z) \geq 0$.

Proof. We assume $\nu \neq k + 1/2$ for integral k and begin by changing variables, $r = |\nu|w$, so that

$$f(z) = \int_0^\infty \frac{\mathrm{Im}\big(u_\nu(|\nu|we^{-\pi i/2})\big)}{iw + z/|\nu|}\, dw = \int_0^\infty \mu_z(w)dw. \tag{4.17}$$

From the nonvanishing of μ_z and its asymptotic behavior in w, it is clear that (4.15) holds for $|\nu| \in (\nu_0, \nu_1)$ and any fixed $\nu_1 > \nu_0$. Using (4.12) for $|\nu|$ large but bounded away from $2k - 1/2$ for integral k, an application of Watson's lemma to (4.14) focuses on the unique positive zero, w^*, of ϕ defined in (3.20). As the derivative of this function is positive, we conclude

$$f(z) \sim \frac{\alpha\cos(\nu\pi)}{iw^* + z/|\nu|}, \tag{4.18}$$

where α is a function of w^*, so that (4.15) clearly holds. However, as $\nu \to 2k - 1/2$, the denominator on the right-hand side of (4.12) may nearly vanish at w^* and the expansion loses its uniformity. Setting $\cos(\nu\pi) = \eta$ in these cases, we see that the denominator has a minimum which is bounded below by $O(\eta^2)$. Hence in an $O(|\nu|^{-1})$ neighborhood of the minimum which includes w^*, we have

$$\int \mu_z(w) \approx \frac{\eta|\nu|\sqrt{1 + (w^*)^2}}{iw^* + z/|\nu|} \int_{-\gamma/|\nu|}^{\gamma/|\nu|} \frac{1}{\eta^2 + \beta^2\nu^2 s^2} ds, \tag{4.19}$$

which by the change of variables $s = \eta z/|\nu|$ is seen to satisfy the upper bound in (4.15) uniformly in η. As the rest of the integral is small, the upper bound holds.

We now move on to the approximation. For a positive integer m and a positive number w_0, we define intervals $I_0 = \big(0, w_0\big)$, $I_j = \big(2^{j-1}w_0, 2^j w_0\big)$ for $j = 1, \ldots, m$, and $I_{m+1} = \big(2^m w_0, \infty\big)$. Now

$$f(z) = f_0(z) + f_1(z) + f_2(z), \tag{4.20}$$

where f_0, f_1, and f_2 are defined by the formulae

(4.21)
$$f_0(z) = \int_{I_0} \mu_z(w)\, dw, \qquad f_1(z) = \sum_{j=1}^{m} \int_{I_j} \mu_z(w)\, dw, \qquad f_2(z) = \int_{I_{m+1}} \mu_z(w)\, dw.$$

We will now choose w_0 and m so that f_0 and f_2 can be ignored and then use Lemma 3.5 to approximate f_1. Using (4.10) and (4.12) and taking w_0 sufficiently small we have, for some constant c_2 independent of ν,

$$|f_0(z)| \le \frac{c_2|\nu|}{1+|z|/|\nu|}\Big(\frac{3e}{4}\Big)^{2|\nu|} \int_0^{w_0} w^{2|\nu|-1} dw \le \frac{c_2}{1+|z|/|\nu|}\Big(\frac{3e}{4}w_0\Big)^{2|\nu|}. \tag{4.22}$$

Hence, a choice of

$$w_0 = O(\varepsilon^{1/(2|\nu|)}), \quad \varepsilon \to 0, \tag{4.23}$$

suffices to guarantee

$$|f_0(z)| \le \frac{\varepsilon}{3}|f(z)| \tag{4.24}$$

in the closed upper half-plane. Now using (4.11) and (4.12) and assuming m sufficiently large we have, for some constant c_3 independent of ν,

$$|f_2(z)| \le \frac{c_3|\nu|}{1+|z|/|\nu|} \int_{2^m w_0}^{\infty} we^{-|\nu|w} dw \le \frac{c_2}{1+|z|/|\nu|} 2^m w_0 e^{-|\nu|2^m w_0}. \tag{4.25}$$

From (4.23), choosing

$$m \ge m_0 + m_1 \frac{1}{|\nu|} \log \frac{1}{\varepsilon} \tag{4.26}$$

for appropriate m_0 and m_1 independent of ν and ε leads to

$$|f_2(z)| \le \frac{\varepsilon}{3}|f(z)|. \tag{4.27}$$

Finally, we apply Lemma 3.5 to the approximation of f_1. The error involves the function $F_1 = \int |\mathrm{Im}(u_\nu)|/(ir+z)dr$, but we note that $|F_1| = |f_1|$. Using p poles for each j we produce a $p \cdot m$-pole approximation $g(z)$ with an error estimate, again for $\mathrm{Im}(z) \ge 0$, given by

$$|f_1(z) - g(z)| \le \frac{5}{3^p - 1}|f_1(z)|. \tag{4.28}$$

A choice of

$$p = O\Big(\log \frac{1}{\varepsilon}\Big) \tag{4.29}$$

enforces

$$|f_1(z) - g(z)| \le \frac{\varepsilon}{3}|f(z)|. \tag{4.30}$$

By combining (4.24), (4.27), (4.30), and the triangle inequality, we obtain (4.16) with the number of poles, $d = p \cdot m$, satisfying the stated bound. ∎

The case $\nu = 0$ requires special treatment. First, the direct application of the preceding arguments leads to a significantly larger upper bound on the number of poles. Second, we note that $u_0(0) = 0$, so that relative error bounds near $z = 0$ require a vanishing absolute error. Finally, the lack of regularity of $u_0(z)$ at $z = 0$ precludes uniform rational approximation, as discussed in [10]. Therefore, we relax the condition $\mathrm{Im}(z) \ge 0$ to $\mathrm{Im}(z) \ge \eta > 0$. By (2.20) this will lead to good approximate convolutions for times $T \le \eta^{-1}$.

LEMMA 4.4. *There exists $\delta > 0$ such that for all ε, $0 < \varepsilon < 1/2$ and η, $0 < \eta < 1/2$, the function $f(z) = u_0(z) - iz + 1/2$ admits an approximation $g(z)$ that is a sum of $d \le \delta \cdot \big(\log(1/\eta) + \log\log(1/\varepsilon)\big) \cdot \log(1/\varepsilon)$ poles, with*

$$|f(z) - g(z)| \le \varepsilon \cdot |f(z)|, \tag{4.31}$$

provided $\mathrm{Im}(z) \ge \eta$.

Proof. Note that since $u_0(z)$ has no poles, $f(z)$ is given by (4.14) and satisfies (4.15). Define intervals

$$I_j = \big((2^{j-1} - 1)\eta, (2^j - 1)\eta\big) \text{ for } j = 1, \dots, m, \quad I_{m+1} = \big((2^m - 1)\eta, \infty\big).$$

Now

$$f(z) = f_1(z) + f_2(z), \tag{4.32}$$

where f_1 and f_2 are defined by the formulae

$$f_1(z) = \sum_{j=1}^{m} \int_{I_j} \frac{\mathrm{Im}(u_0(re^{-\pi i/2}))}{ir + z}\, dr, \qquad f_2(z) = \int_{I_{m+1}} \frac{\mathrm{Im}(u_0(re^{-\pi i/2}))}{ir + z}\, dr. \tag{4.33}$$

We will now choose m so that f_2 can be ignored and then use Lemma 3.5 to approximate f_1. Using (4.11) and assuming m sufficiently large we have, for some constant c,

$$|f_2(z)| \le \frac{c}{1 + |z|} \int_{(2^m - 1)\eta}^{\infty} re^{-2r} dw \le \frac{c}{1 + |z|} 2^{m-1} \eta e^{-2^m \eta}. \tag{4.34}$$

Hence, choosing

$$m \ge m_0\big(\log(1/\eta) + \log\log(1/\varepsilon)\big) \tag{4.35}$$

for appropriate m_0 independent of η and ε leads to

$$|f_2(z)| \le \frac{\varepsilon}{2}|f(z)|. \tag{4.36}$$

Finally, we apply Lemma 3.5 to the approximation of f_1. Using p poles for each j we produce a $p \cdot m$-pole approximation $g(z)$ with an error estimate for $\mathrm{Im}(z) \geq \eta$ given by

$$|f_1(z) - g(z)| \leq \frac{5}{3^p - 1}|f_1(z)|. \tag{4.37}$$

A choice of

$$p = O\Big(\log \frac{1}{\varepsilon}\Big) \tag{4.38}$$

enforces

$$|f_1(z) - g(z)| \leq \frac{\varepsilon}{2}|f(z)|. \tag{4.39}$$

By (4.36), (4.39), and the triangle inequality, (4.31) is achieved with the number of poles, $d = p \cdot m$, satisfying the stated bound. □

We now consider the contribution of the poles.

LEMMA 4.5. *There exist constants C_0, C_1, $\delta > 0$ such that for all $\nu, \varepsilon \in \mathbb{R}$ with $2 \leq |\nu|$ and $0 < \varepsilon < 1/2$ the function*

$$h(z) = \sum_{n=1}^{N_\nu} \frac{h_{\nu,n}}{z - h_{\nu,n}}, \tag{4.40}$$

where $h_{\nu,1}, \ldots, h_{\nu,N_\nu}$ are the roots of $H_\nu^{(1)}$, satisfies the inequalities

$$\frac{C_1|\nu|}{1 + |z|/|\nu|} \leq |h(z)| \leq \frac{C_2|\nu|}{1 + |z|/|\nu|}, \tag{4.41}$$

and admits an approximation $g(z)$ that is a sum of $d \leq \delta \cdot \log|\nu| \cdot \log(1/\varepsilon)$ poles, with

$$|h(z) - g(z)| \leq \varepsilon \cdot |h(z)|, \tag{4.42}$$

provided $\mathrm{Im}(z) \geq 0$.

Proof. The curve C defined in Lemma 3.2, near which $h_{\nu,1}/|\nu|, \ldots, h_{\nu,N_\nu}/|\nu|$ lie, is contained in disks separated from the real axis. If we denote the disk of radius r centered at c by $D(r, c)$, then the disks

$$\big\{ D(-\mathrm{Im}(z), z) \big|\ z \in C, |\arg z - \pi/2| = \pi/2 + \pi/2^n,\ n = 1, 2, \ldots \big\}, \tag{4.43}$$

for example, contain $C \backslash \{+1, -1\}$. From (3.31), the root $h_{\nu,1}$ closest to the real axis satisfies

$$\arg h_{\nu,1} \sim \frac{a_1\sqrt{3}}{2^{4/3}}|\nu|^{-2/3}; \tag{4.44}$$

hence it is contained in a disk of (4.43) with $n \approx \log_2\big(2^{4/3}3^{-1/2}\pi(-a_1)^{-1}|\nu|^{2/3}\big)$, and all of the roots are contained in $O(\log|\nu|)$ of the disks. Now applying Lemma 3.4 we obtain (4.42) with $|h|$ replaced by $|H| = \big|\sum |h_{\nu,n}|/(z - h_{\nu,n})\big|$. To obtain the upper bound in (4.41) for both h and H we note first that it is trivial except for $|z/\nu| \approx 1$. A detailed analysis of the roots as described by Lemma 3.2 shows that

$$\big|\mathrm{Im}(h_{\nu,j})\big| \geq cj^{2/3}|\nu|^{1/3}. \tag{4.45}$$

Hence, for $|z/\nu| \approx 1$,

$$\sum_j \Big| \frac{h_{\nu,j}}{z - h_{\nu,j}} \Big| \le C|\nu|^{2/3} \sum_{j=1}^{|\nu|} j^{-2/3} \le 3C|\nu|. \tag{4.46}$$

The lower bound in (4.41) is again obvious except for $|z/\nu| \approx 1$. Then, however, we note that

$$h(z) = u_\nu(z) - iz + 1/2 - f(z). \tag{4.47}$$

Since, from (3.26), $|u_\nu(z)| = O(|\nu|^{2/3})$ for $|z/\nu| \approx 1$ and $|f(z)| = O(1)$ by (4.15) the right-hand side is dominated by $-iz$ and $|h(z)| = O(|\nu|)$. ∎

The combination of Theorem 4.1 and Lemmas 4.3 and 4.5 suffices to prove our principal analytical result.

THEOREM 4.6. *Given $\nu_0 > 0$ there exists $\delta > 0$ such that for all $\nu \in \mathbb{R}$, $|\nu| \ge \nu_0$, and $0 < \varepsilon < 1/2$ there exists d with*

$$d \le \delta\big(\log|\nu| \cdot \log(1/\varepsilon) + \log^2|\nu| + |\nu|^{-1} \log^2(1/\varepsilon) \big), \tag{4.48}$$

and complex numbers $\alpha_1, \dots, \alpha_d$ and $\beta_1, \dots, \beta_d$, depending on ν and ε, such that the function

$$U_{\nu,\varepsilon}(z) = iz - \frac{1}{2} + \sum_{n=1}^{d} \frac{\alpha_n}{z - \beta_n} \tag{4.49}$$

approximates $u_\nu(z)$ with the bound

$$\big| u_\nu(z) - U_{\nu,\varepsilon}(z) \big| \le \varepsilon \cdot \big| u_\nu(z) \big|, \tag{4.50}$$

provided that $\mathrm{Im}(z) \ge 0$. *Furthermore*

$$\left(\int_{-\infty}^{\infty} \big| u_\nu(x) - U_{\nu,\varepsilon}(x) \big|^2 dx \right)^{1/2} \le \varepsilon \cdot \left(\int_{-\infty}^{\infty} \big| u_\nu(x) - ix + 1/2 \big|^2 dx \right)^{1/2}. \tag{4.51}$$

Proof. We first note the lower bound

$$\big| u_\nu(z) - iz + 1/2 \big| \ge \frac{c|\nu|}{1 + |z|/|\nu|}. \tag{4.52}$$

For $\nu > 0$ the function is nonvanishing and has the correct asymptotic behavior, so we need only consider the case of $|\nu|$ large. The result then follows from (3.26). This proves (4.51) and (4.50) with u_ν replaced by $u_\nu - iz + 1/2$ on the right-hand side. From (3.26) we have

$$\big| u_\nu(z) - iz + 1/2 \big| \le c|\nu|^{1/3} \big| u_\nu(z) \big|, \tag{4.53}$$

so that the final result follows from the scaling $\varepsilon \to |\nu|^{-1/3}\varepsilon$. ∎

The number of poles in (4.48) required to approximate $u_\nu(z)$ to a tolerance ε depends on both ε and ν. The asymptotic dependence on ε is proportional to $|\nu|^{-1} \log^2(1/\varepsilon)$. We will see in the numerical examples, however, that this term is important only for small $|\nu|$; otherwise the dominant term is the first, for an asymptotic

dependence of $O\big(\log|\nu|\cdot\log(1/\varepsilon)\big)$. As we generally have $\varepsilon \ll |\nu|^{-1}$ in practice, the term $\log^2|\nu|$ is of less importance.

Similarly, Lemma 4.4 leads to the following theorem for $\nu = 0$.

THEOREM 4.7. *There exists $\delta > 0$ such that for all ε, $0 < \varepsilon < 1/2$ and η, $0 < \eta < 1/2$ there exists $d \le \delta \cdot \big(\log(1/\eta)\cdot\log(1/\varepsilon) + \log\log(1/\varepsilon) + \log\log(1/\eta)\big)$ and complex numbers $\alpha_1, \ldots, \alpha_d$ and $\beta_1, \ldots, \beta_d$, depending on η and ε, such that the function*

$$U_{0,\varepsilon}(z) = iz - \frac{1}{2} + \sum_{n=1}^{d} \frac{\alpha_n}{z - \beta_n} \tag{4.54}$$

approximates $u_0(z)$ with the bound

$$\big|u_0(z) - U_{0,\varepsilon}(z)\big| \le \varepsilon \cdot \big|u_0(z)\big|, \tag{4.55}$$

provided that $\mathrm{Im}(z) \ge \eta$. *Furthermore*

$$\left(\int_{-\infty}^{\infty} \big|u_0(x+i\eta) - U_{0,\varepsilon}(x+i\eta)\big|^2 dx\right)^{1/2} \le \varepsilon \cdot \left(\int_{-\infty}^{\infty} \big|u_\nu(x+i\eta) - ix + \eta + 1/2\big|^2 dx\right)^{1/2}. \tag{4.56}$$

Proof. Again we already have (4.55) with $u_0(z) - iz + 1/2$ on the right-hand side. By (3.24) we find

$$\big|u_0(z) - iz + 1/2\big| \le c\log(1/\eta)\big|u_0(z)\big|. \tag{4.57}$$

The theorem follows from the scaling $\varepsilon \to \log^{-1}(1/\eta)\varepsilon$. ∎

As we must take $\eta = T^{-1}$, we see that the number of poles required may grow like $\log(1/\varepsilon)\cdot\log T + \log T\cdot\log\log T$. However, this is only for the mode $n = 0$ in the two-dimensionsal case. In short, the T dependence is insignificant in practice.

5. Computation of the rational representations. Analytical error bound estimates developed in the previous sections are based on maximum norm errors as in (2.19) and (2.20). In numerical computation it is often convenient, however, to obtain least squares solutions. Our method of computing a rational function $U_{\nu,\varepsilon}$ that satisfies (4.50) is to enforce (4.51). An alternative approach would be to use rational Chebyshev approximation as developed by Trefethen and Gutknecht [24, 25, 26].

In the numerical computations, we work with

$$\tilde{u}_\nu(z) = u_\nu(z) - iz + 1/2 \tag{5.1}$$

and its sum-of-poles approximation $\tilde{U}_{\nu,\varepsilon}(z) = U_{\nu,\varepsilon}(z) - iz + 1/2$. In particular, we have the nonlinear least squares problem

$$\min_{P,Q} \int_{-\infty}^{\infty} \left|\frac{P(x)}{Q(x)} - \tilde{u}_\nu(x)\right|^2 dx \tag{5.2}$$

for P, Q polynomials with $\deg(P) + 1 = \deg(Q) = d$. Problem (5.2) is not only nonlinear, but also very poorly conditioned when P, Q are represented in terms of

their monomial coefficients. We apply two tactics for coping with these difficulties: linearization and orthogonalization.

We linearize the problem by starting with a good estimate of Q and updating P, Q iteratively. In particular, we solve the linear least squares problem

$$\min_{P^{(i+1)},Q^{(i+1)}} \int_{-\infty}^{\infty} \Big| \frac{P^{(i+1)}(x)}{Q^{(i)}(x)} - \frac{Q^{(i+1)}(x)}{Q^{(i)}(x)}\, \tilde{u}_\nu(x) \Big|^2 dx, \tag{5.3}$$

where the integral is replaced by a quadrature. The initial values $P^{(0)}$, $Q^{(0)}$ are obtained by exploiting the asymptotic expansion (3.25) and the recurrence (3.28). We find that two to three iterations of (5.3) generally suffice.

The quadrature for (5.3) is derived by first changing variables,

$$\int_{-\infty}^{\infty} f(x)\, dx = \int_{-\pi/2}^{\pi/2} f(\tan\theta)\, \sec^2\theta\, d\theta \approx \sum_{i=1}^{m} w_i\, f(\tan\theta_i)\, \sec^2\theta_i, \tag{5.4}$$

where $\theta_1, \ldots, \theta_m$ and $w_1 \ldots, w_m$ denote appropriate quadrature nodes and weights. The transformed integrand is periodic on the interval $[-\pi/2, \pi/2]$, so the trapezoidal rule (or midpoint rule) is an obvious candidate. The integrand is infinitely continously differentiable, except at $\theta = 0$, where its regularity is of order $2|\nu|$. For $|\nu| > 8$ (say), the trapezoidal rule delivers at least 16th-order convergence and is very effective. For small $|\nu|$, however, a quadrature that adjusts for the complicated singularity at $\theta = 0$ is needed. Here we can successively subdivide the interval near the singularity, applying high-order quadratures on each subinterval (see, for example, [27]).

The quadrature discretization of (5.3) cannot be solved as a least squares problem by standard techniques, due to its extremely poor conditioning. We avoid forming the corresponding matrix; rather we solve the least squares problem by Gram–Schmidt orthogonalization. The $2d + 1$ functions

$$\tilde{u}_\nu,\ 1,\ x\tilde{u}_\nu,\ x, \ldots, x^{d-1}\tilde{u}_\nu,\ x^{d-1},\ x^d\tilde{u}_\nu \tag{5.5}$$

are orthogonalized under the real inner product

$$\langle f, g\rangle_i = \int_{-\infty}^{\infty} \frac{\mathrm{Re}\big(f(x)\,\bar{g}(x)\big)}{\big|Q^{(i)}(x)\big|^2}\, dx \tag{5.6}$$

to obtain the orthogonal functions

$$g_n(x) = \begin{cases} \tilde{u}_\nu(x), & n = 1, \\ 1, & n = 2, \\ x g_{n-2}(x) - \sum_{j=1}^{\min\{4,n-1\}} c_{nj}\, g_{n-j}(x), & n = 3, \ldots, 2d+1, \end{cases} \tag{5.7}$$

where

$$c_{nj} = \frac{\langle x g_{n-2}, g_{n-j}\rangle_i}{\langle g_{n-j}, g_{n-j}\rangle_i}, \qquad \begin{matrix} n = 3, \ldots, 2d+1, \\ j = 1, \ldots, \min\{4, n-1\}. \end{matrix} \tag{5.8}$$

Now

$$g_{2d+1} = -P^{(i+1)} + \tilde{u}_\nu\, Q^{(i+1)}, \tag{5.9}$$

TABLE 1

Number d of poles to represent the Laplace transform of nonreflecting boundary kernels σ_n and ω_n, for various values of ε.

$\varepsilon = 10^{-6}$			
σ_n		ω_n	
n	d	n	d
0	26		
1	9		
2	6		
3– 6	5	0– 5	n
7– 8	6	6– 8	6
9– 12	7	9– 12	7
13– 19	8	13– 19	8
20– 31	9	20– 31	9
32– 51	10	32– 51	10
52– 86	11	52– 86	11
87– 147	12	87– 147	12
148– 227	13	148– 228	13
228– 401	14	229– 402	14
402– 728	15	403– 728	15
729–1024	16	729–1024	16

$\varepsilon = 10^{-8}$			
σ_n		ω_n	
n	d	n	d
0	44		
1	15		
2	9		
3– 8	7	0– 7	n
9– 10	8	8– 10	8
11– 14	9	11– 14	9
15– 20	10	15– 19	10
21– 28	11	20– 28	11
29– 41	12	29– 40	12
42– 58	13	41– 57	13
59– 84	14	58– 83	14
85– 123	15	84– 123	15
124– 183	16	124– 183	16
184– 275	17	184– 275	17
276– 418	18	276– 418	18
419– 638	19	419– 637	19
639– 971	20	638– 971	20
972–1024	21	972–1024	21

$\varepsilon = 10^{-15}$			
σ_n		ω_n	
n	d	n	d
1	41		
2	24		
3	18		
4	15		
5	14		
6	13		
7– 12	12		
13– 14	13	0– 13	n
15– 16	14	14– 15	14
17– 18	15	16– 18	15
19– 22	16	19– 21	16
23– 26	17	22– 25	17
27– 31	18	26– 30	18
32– 37	19	31– 36	19
38– 45	20	37– 44	20
46– 54	21	45– 53	21
55– 65	22	54– 65	22
66– 79	23	66– 79	23
80– 97	24	80– 96	24
98– 118	25	97– 118	25
119– 145	26	119– 144	26
146– 177	27	145– 176	27
178– 216	28	177– 216	28
217– 265	29	217– 264	29
266– 324	30	265– 324	30
325– 397	31	325– 396	31
398– 486	32	397– 485	32
487– 595	33	486– 594	33
596– 728	34	595– 727	34
729– 890	35	728– 890	35
891–1024	36	891–1024	36

so $P^{(i+1)}$ and $Q^{(i+1)}$ are computed from the recurrence coefficients c_{nj} by splitting (5.7) into even- and odd-numbered parts.

For some applications, including nonreflecting boundary kernels, it is convenient to represent P/Q as a sum of poles,

$$\frac{P(z)}{Q(z)} = \sum_{n=1}^{d} \frac{\alpha_n}{z - \beta_n}. \tag{5.10}$$

We compute $\beta_1, \ldots, \beta_d$ (zeros of Q) by Newton iteration with zero suppression (see,

TABLE 2

Laplace transform of cylinder kernel σ_n defined in (2.13), approximated as a sum of d poles, for $n = 1, \ldots, 4$ and $\varepsilon = 10^{-6}$.

		Pole Coefficient		Pole Location	
n	d	Re	Im	Re	Im
1	9	$-0.426478E-02$	$0.000000E+00$	$-0.368403E+01$	$0.000000E+00$
		$-0.416255E-01$	$0.000000E+00$	$-0.205860E+01$	$0.000000E+00$
		$-0.122665E+00$	$0.000000E+00$	$-0.118994E+01$	$0.000000E+00$
		$-0.143704E+00$	$0.000000E+00$	$-0.717570E+00$	$0.000000E+00$
		$-0.530662E-01$	$0.000000E+00$	$-0.423506E+00$	$0.000000E+00$
		$-0.863872E-02$	$0.000000E+00$	$-0.223111E+00$	$0.000000E+00$
		$-0.961472E-03$	$0.000000E+00$	$-0.103710E+00$	$0.000000E+00$
		$-0.721548E-04$	$0.000000E+00$	$-0.409342E-01$	$0.000000E+00$
		$-0.250102E-05$	$0.000000E+00$	$-0.117156E-01$	$0.000000E+00$
2	6	$0.218164E-01$	$0.000000E+00$	$-0.333263E+01$	$0.000000E+00$
		$0.860648E+00$	$0.000000E+00$	$-0.162945E+01$	$0.000000E+00$
		$-0.138934E+01$	$0.162069E+00$	$-0.125843E+01$	$0.412637E+00$
		$-0.138934E+01$	$-0.162069E+00$	$-0.125843E+01$	$-0.412637E+00$
		$0.209905E-01$	$0.000000E+00$	$-0.612710E+00$	$0.000000E+00$
		$0.232032E-03$	$0.000000E+00$	$-0.240327E+00$	$0.000000E+00$
3	5	$-0.179277E+00$	$0.000000E+00$	$-0.309775E+01$	$0.000000E+00$
		$-0.168335E+01$	$0.129111E+01$	$-0.167998E+01$	$0.130784E+01$
		$-0.168335E+01$	$-0.129111E+01$	$-0.167998E+01$	$-0.130784E+01$
		$-0.816322E+00$	$0.000000E+00$	$-0.187260E+01$	$0.000000E+00$
		$-0.126962E-01$	$0.000000E+00$	$-0.950854E+00$	$0.000000E+00$
4	5	$-0.197725E+01$	$0.220886E+01$	$-0.197861E+01$	$0.220444E+01$
		$-0.197725E+01$	$-0.220886E+01$	$-0.197861E+01$	$-0.220444E+01$
		$-0.219247E+01$	$0.216535E+01$	$-0.282304E+01$	$0.382237E+00$
		$-0.219247E+01$	$-0.216535E+01$	$-0.282304E+01$	$-0.382237E+00$
		$0.464435E+00$	$0.000000E+00$	$-0.201159E+01$	$0.000000E+00$

for example, [28]) by the formula

$$\beta_n^{(j+1)} = \beta_n^{(j)} - \frac{Q\big(\beta_n^{(j)}\big)}{Q'\big(\beta_n^{(j)}\big) - \displaystyle\sum_{k=1}^{n-1} \frac{Q\big(\beta_n^{(j)}\big)}{\beta_n^{(j)} - \beta_k}}, \tag{5.11}$$

where $\beta_1, \ldots, \beta_{n-1}$ are the previously computed zeros of Q. Then $\alpha_1, \ldots, \alpha_d$ are computed by the formula $\alpha_n = P(\beta_n)/Q'(\beta_n)$. The derivative $Q'(z)$ is obtained by differentiating the recurrence (5.7).

6. Numerical results. We have implemented the algorithm described in section 5 to compute the representations of σ_n and ω_n through their Laplace transforms. Recall that for the cylinder kernels, σ_n, we have $\nu = n$ while for the sphere kernels, ω_n, we have $\nu = n + 1/2$. Table 1 presents the sizes of the representations for $\varepsilon = 10^{-6}$, 10^{-8}, and 10^{-15} in (4.51). For the cylinder kernels, which are affected by the branch cut, the number of poles for small n is higher than for the sphere kernels. This discrepancy, however, rapidly vanishes as n increases and the asymptotic performance ensues. The $\log(1/\varepsilon)$ dependence of the number of poles for $n \geq 10$ is clear.

For $\varepsilon = 10^{-8}$ we have also computed the maximum norm relative errors which appear in (2.19) by sampling on a fine mesh. For the cylinder kernel with $n = 0$, we expect an $O(1)$ error in a small interval about the origin due to (4.10). However, errors of less than ε are achieved for $|s| > 5 \times 10^{-7}$. This implies a similar accuracy in the approximation of the convolution for times of order 10^6. For all other cases the maximum norm relative errors are of order ε.

Finally, Table 2 presents poles and coefficients for the cylinder kernels for $n = 1, \ldots, 4$ and $\varepsilon = 10^{-6}$ to allow comparison by a reader interested in repeating our calculations. Note that the pole locations are written in terms of $s = z/i$. Extensive tables will be made available on the Web at http://math.nist.gov/mcsd/Staff/BAlpert.

Remark. Our approximate representation of the nonreflecting boundary kernel could be used to reduce the cost of the method introduced by Grote and Keller [8]. The differential operators of degree n obtained in their derivation need only be replaced by the corresponding differential operators of degree $\log n$ for any specified accuracy. It is interesting to note that in the two-dimensional case, where the approach of [8] does not apply, the analysis described above can be used to derive an integrodifferential formulation in the same spirit.

7. Summary. In this paper we have introduced new representations for the logarithmic derivative of a Hankel function of real order, that scale in size as the logarithm of the order. An algorithm to compute the representations was presented and our numerical results demonstrate that the new representations are modest in size for orders and accuracies likely to be of practical interest.

The present motivation for this work is the numerical modeling of nonreflecting boundaries for the wave equation, discussed briefly here and in more detail in [18]. Maxwell's equations are also susceptible to similar treatment as outlined in [29]. The new representations enable the application of the exact nonreflecting boundary conditions, which are global in space and time, to be computationally effective.

8. Appendix: Stability of exact and approximate conditions. In this appendix, we consider the stability of our approach to the design of nonreflecting boundary conditions. Given that we are approximating the exact conditions uniformly, it is natural to expect that our approximations possess similar stability characteristics. This is, indeed, the case. Oddly enough, however, the exact boundary conditions themselves do *not* satisfy the uniform Kreiss–Lopatinski conditions which are necessary and sufficient for strong well-posedness in the usual sense [30]. This may seem paradoxical since the unbounded domain problem itself is strongly well-posed. The difficulty is that the exact reduction of an unbounded domain problem to a bounded domain problem gives rise to forcings (inhomogeneous boundary terms) which live in a restricted subspace. The Kreiss–Lopatinski conditions, on the other hand, require bounds for arbitrary forcings. In that setting, our best estimates result in the loss of 1/3 of a derivative in terms of Sobolev norms. In practice we doubt that this fact is of any significance, and have certainly encountered no stability problems in our long time numerical simulations.

To fill in some of the details, consider a spherical domain Ω of radius one, within which the homogeneous wave equation with homogeneous initial data is satisfied. At the boundary we have

$$\frac{\partial \hat{u}_{nm}}{\partial r} = (1 + \epsilon_n(s)) \frac{s k_n'(s)}{k_n(s)} \hat{u}_{nm} + \hat{g}_{nm}, \tag{8.1}$$

where $\epsilon_n = 0$ for the exact condition and is uniformly small when we use our approximations. Here $\hat{g}_{nm}$ is the spherical harmonic transform of an arbitrary forcing g.

Following Sakamoto, we seek to estimate

$$\mathcal{H}(u) = \int_0^T \left(\|u(\cdot,t)\|_{1,\Omega}^2 + \|u(\cdot,t)\|_{1,\partial\Omega}^2 + \left\| \frac{\partial u}{\partial r}(\cdot,t) \right\|_{0,\partial\Omega}^2 \right) dt, \tag{8.2}$$

where

$$\|f\|_{1,\Omega}^2 = \int_\Omega \left(f^2 + |\nabla f|^2\right), \tag{8.3}$$

while $\|\cdot\|_{0,\Omega}$ denotes the usual L_2 norm. On the boundary, $\partial\Omega$, we will make use of fractional Sobolev norms, most easily defined in terms of the spherical harmonic coefficients:

$$\|f\|_{p,\partial\Omega}^2 = \sum_{n,m}(1+n^2)^p|\hat{f}_{nm}|^2. \tag{8.4}$$

Strong well-posedness would follow from showing that

$$\mathcal{H}(u) \le c\int_0^T \|g(\cdot,t)\|_{0,\partial\Omega}^2 dt. \tag{8.5}$$

Instead, we can show that

$$\mathcal{H}(u) \le c\int_0^T \|g(\cdot,t)\|_{1/3,\partial\Omega}^2 dt. \tag{8.6}$$

To prove this, let $s = iz$ and note that

$$k_n(s) \propto h_n^{(1)}(z) \propto z^{-1/2}H_\nu^{(1)}(z), \quad \nu = n + \frac{1}{2}. \tag{8.7}$$

Bounded solutions within the sphere are given by

$$\hat{u}_{nm}(r,s) \propto j_n(rz) \propto (rz)^{-1/2}J_\nu(rz). \tag{8.8}$$

Precisely, setting

$$\hat{u}_{nm}(r,s) = A_{nm}(z)(rz)^{-1/2}J_\nu(rz), \tag{8.9}$$

we find

$$A_{nm}(z) = -\frac{2i}{\pi}z^{1/2}H_\nu^{(1)}(z)\delta_n(z)\hat{g}_{nm}(z), \tag{8.10}$$

where

$$\delta_n = \left(1 - \frac{\pi i}{2}\epsilon_n J_\nu(z)(zH_\nu^{(1)\prime}(z) - \frac{H_\nu^{(1)}(z)}{2})\right)^{-1}. \tag{8.11}$$

We now estimate norms of the solution. First note that the products in the definition of δ_n, $J_\nu(z)H_\nu^{(1)}(z)$, $zJ_\nu(z)H_\nu^{(1)\prime}(z)$, are uniformly bounded for $\mathrm{Im}(z) \ge 0$. (See the limits $z \to 0$, $z \to \infty$, and $\nu \to \infty$.) Therefore, as mentioned above, the error term, so long as it's small, has no effect on the estimates we derive, and we simply ignore it. That is, we set $\delta_n = 1$.

We concentrate on the boundary terms in $\mathcal{H}$, as they are both the most straightforward to compute and the most ill behaved. In transform space we have

$$(1+n^2)|\hat{u}_{nm}(1,s)|^2 + |s\hat{u}'_{nm}(1,s)|^2 \le c\gamma_\nu^2(z)|\hat{g}_{nm}(z)|^2, \tag{8.12}$$

$$\gamma_\nu^2(z) = |H_\nu^{(1)}(z)|^2 \left(\nu^2 |J_\nu(z)|^2 + |z|^2 |J_\nu'(z)|^2\right). \tag{8.13}$$

(Here and throughout, c will denote a positive constant independent of all variables.) We first note that as the only singularities of Bessel functions occur at zero and infinity, we need only consider the limits $z \to 0$, $z \to \infty$, and $\nu \to \infty$. The first two are straightforward:

$$\gamma_\nu^2(z) \approx c\Gamma^2(\nu)(z/2)^{-2\nu} \left(\nu^2 (z/2)^{2\nu}/\Gamma^2(\nu+1)\right) = c, \quad z \to 0, \tag{8.14}$$

$$\gamma_\nu^2(z) \approx c|z|^{-1} \left(\nu^2 |z|^{-1} \cos^2 z + |z| \sin^2 z\right) \approx c \sin^2 z, \quad z \to \infty. \tag{8.15}$$

For large ν we use the uniform asymptotic expansions of Bessel functions due to Olver [20], which yield

$$\sup_z \gamma_\nu^2(z) = O(\nu^{2/3}). \tag{8.16}$$

From Parseval's relation, we conclude that

$$\int_0^T \left(\|u(\cdot,t)\|_{1,\partial\Omega}^2 + \left\| \frac{\partial u}{\partial r}(\cdot,t) \right\|_{0,\partial\Omega}^2 \right) dt \le c \int_0^T \|g(\cdot,t)\|_{1/3,\partial\Omega}^2 dt. \tag{8.17}$$

The estimation of the spatial integrals is more involved, as for $r < 1$ the solution has two transition zones, $z \approx \nu$ and $rz \approx \nu$, and there are a number of cases to consider. However, the estimates follow along the same lines and lead to the same result.

It is interesting to note that the loss-of-derivative phenomenon is suppressed when one looks at the error due to the approximation of the boundary condition. In that case the transform of the exact solution near the boundary is

$$\frac{h_n^{(1)}(rz)}{h_n^{(1)}(z)} \hat{u}_{nm}(1,s), \tag{8.18}$$

so that the error, e, satisfies the problem above with $\hat{g}_{nm}$ given by

$$\hat{g}_{nm} = \epsilon_n \frac{z h_n^{(1)'}(z)}{h_n^{(1)}(z)} \hat{u}_{nm}(1,s) \equiv \epsilon_n \mu_n(z) \hat{u}_{nm}(1,s). \tag{8.19}$$

Now the best estimate of μ_n takes the form

$$|\mu_n| \le c(|z| + \nu), \tag{8.20}$$

which, in combination with (8.6), would lead to an estimate of the 1-norms of the error in terms of the 4/3-norms of the solution. However, using again the large ν asymptotics, a direct calculation shows

$$|\mu_n \gamma_\nu| \le c(|z| + \nu). \tag{8.21}$$

Thus μ_n is smaller than its maximum by $O(\nu^{-1/3})$ in the transition region where $\gamma_\nu = O(\nu^{1/3})$. Hence we find for the error

$$\mathcal{H}(e) \le c \sup_{n,s} |\epsilon_n|^2 \int_0^T \left(\|u(\cdot,t)\|_{1,\partial\Omega}^2 + \left\| \frac{\partial u}{\partial t}(\cdot,t) \right\|_{0,\partial\Omega}^2 \right) dt. \tag{8.22}$$

In other words, the 1-norms of the error are controlled by the 1-norms of the solution.

We have, of course, ignored discretization error, which could conceivably cause difficulties in association with the lack of strong well-posedness. To rule them out would require a more detailed analysis. In practice we have encountered no difficulties, even for very long time simulations. We should also note that strong well-posedness could be artificially recovered by perturbing the approximate conditions for large n. allowing high accuracy to be maintained for smooth solutions. Finally, we note that a similar analysis can be carried out in two dimensions.

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