FAST SOLVERS OF THE LIPPMANN-SCHWINGER EQUATION

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Abstract. *The electromagnetic and acoustic scattering problems for the Helmholz equation in two and three dimensions are equivalent to the Lippmann-Schwinger equation which is a weakly singular volume integral equation on the support of the scatterer. We propose for the Lippmann-Schwinger equation two discretizations of the optimal accuracy order, accompanied by fast solvers of corresponding systems of linear equations. The first method is of the second order and based on simplest cubatures; the scatterer is allowed to be only piecewise smooth. The second method is of arbitrary order and is based on a fully discrete version of the collocation method with trigonometric test functions; the scatterer is assumed to be smooth on whole space* $\mathbb{R}^n$ *and of compact support.*

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1 Introduction

In this paper we deal with the integral equation formulation on the scattering problem for the Helmholtz equation in the inhomogeneous media. We assume that the inhomogeneity is smooth or piecewise smooth and of compact support containing the origin, with possibly complex-valued smooth or piecewise smooth refractive index $b : \mathbb{R}^n \to \mathbb{C}$, $n = 2$ or 3, $b(x) = 1$ outside the inhomogeneity. The formulation of the problem reads as follows: find $u : \mathbb{R}^n \to \mathbb{C}$ ($n = 2$ or 3) such that

$$\Delta u(x) + \kappa^2 b(x) u(x) = 0\,, \qquad x \in \mathbb{R}^n, \tag{1}$$

$$u = u^i + u^s, \tag{2}$$

$$\lim_{r=|x|\to\infty} r^{(n-1)/2}\Big(\frac{\partial u^s}{\partial r} - i\kappa u^s\Big) = 0 \quad \text{uniformly for} \quad \frac{x}{|x|} \in S(0,1) \tag{3}$$

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where u^i (the incident field) is a given entire solution of the Helmholtz equation $\Delta u + \kappa^2 u = 0$, $x \in \mathbb{R}^n$ (usually u^i is given as a plain wave: $u^i(x) = \exp(i\kappa d \cdot x)$, $d \in \mathbb{R}^n$, $|d| = 1$), u^s is the scattered field, $\kappa > 0$ is the wave number; (3) means that u^s must satisfy the Sommerfeld radiation condition. We refer to [2] for more details concerning problem (1)–(3).

Problem (1)–(3) is equivalent to the Lippmann–Schwinger integral equation (see [2])

$$u(x) = u^i(x) - \kappa^n \int_{\mathbb{R}^n} \Phi(\kappa|x-y|)a(y)u(y)dy \tag{4}$$

where $a = 1 - b$ is smooth or piecewiese smooth and of compact support,

$$\Phi(r) = \left\{ \begin{array}{ll} \frac{i}{4} H_0^{(1)}(r), & n = 2 \\ \frac{1}{4\pi}\frac{e^{ir}}{r} \quad , & n = 3 \end{array} \right\}, \quad r > 0\,, \tag{5}$$

$H_0^{(1)}$ is the Hankel funktion of the first kind of order zero (see [1], formula 9.1.3). For $r \to 0$, $H_0^{(1)}(r) \sim -\frac{1}{2\pi}\ln r$. Thus integral equation (4) is weakly singular both in cases $n = 2$ and $n = 3$. The integration over $\mathbb{R}^n$ can be replaced by the integration over $\operatorname{supp} a$.

Problem (1)–(3) and integral equation (4) are uniquely solvable if and only in the homogeneous integral equation corresponding to (4) has only the trivial solution or, equivalently, the homogeneous problem corresponding to, (1)–(3), i.e. the problem with $u^i = 0$, has only the trivial solution.

The unboundedness of the domain $\mathbb{R}^n$ in problem (1)–(3) causes some numerical difficulties. A simplest idea is to use grid methods in a large ball $B(0, R)$, with boundary condition $\frac{\partial u^s}{\partial r} - i\kappa u^s = 0$ for $|x| = R$. This method produces very large discrete problems. Another, more popular idea elaborated in [5] is to use coupled finite and boundary methods: in a ball $B(0, \varrho)$ containing the support of $a = 1 - b$, the problem is treated by finite elements; a boundary integral equation and the Nystrom method are used to treat the problem in the domain $|x| > \varrho$; finally, a special equation is derived to produce appropriate boundary values of $u + i\kappa\frac{\partial u}{\partial r}$ for $|x| = \varrho$. This approach is complicated in it essence. As mentioned in [2], the volume potential approach, i.e. the solution of Lippmann–Schwinger equation (4) instead of (1)–(3), has the advantage that the problem in an unbounded domain is handled in a simple and natural way; a disadvantage is that one has to approximate multidimensional weakly singular integrals and that the discrete problem derived from (4) has a non-sparse matrix. In the present paper we try to show that actually these disadvantages are not serious. First, the optimal convergence order

$$\|v_N - au\|_\lambda \le cN^{\lambda-\mu}\|au\|_\mu \qquad (0 \le \lambda \le \mu)$$

in the scale of Sobolev norms with any $\mu > n/2$ can be achieved by trigonometric collocation method (cf. [6]) applied to a periodized version of (4) if a and u^i are sufficiently smooth ($a \in W^{\mu,2}(\mathbb{R}^n)$ and $u^i \in W^{\mu,2}_{loc}(\mathbb{R}^n)$). Secondly, the N^n parameters of v_N can be computed in $\mathcal{O}(N^n \ln N)$ arithmetical operations. Finally, the algorithm needs to store $\mathcal{O}(N^n)$ quantities. The method is treated in Section 3. In Section 2 we discuss a method of the second accuracy order:

$$\max_j |u_{j,h} - u(jh)| \le ch^2(1 + |\ln h|)\,, \qquad h = 1/N\,;$$

here a may be only piecewise smooth. This method is a modification of a simplest cubature formula method examined in [7] for more general weakly singular integral equations. The purpose of the modification is to obtain a convolution system as the discrete counterpart of (4) maintaining the second order of the approximation. The convolution system can be solved in $\mathcal{O}(N^n \log N)$ arithmetical operations using FFT and two grid iterations.

2 The case of piecewise smooth a

First we somewhat simplify the form of the integral equation (4). The change of variables

$$\tilde{x} = \kappa x\,, \quad \tilde{y} = \kappa y\,, \quad \tilde{u}(\tilde{x}) = u(x)\,, \quad \tilde{a}(\tilde{y}) = a(y)\,, \quad \tilde{u}^i(\tilde{x}) = u^i(x)$$

transforms (4) into

$$\tilde{u}(\tilde{x}) = \tilde{u}^i(\tilde{x}) - \int_{\mathbb{R}^n} \Phi(|\tilde{x} - \tilde{y}|)\tilde{u}(\tilde{y})d\tilde{y}$$

which is (4) with $\kappa = 1$. Thus, without a loss of generality, we put $\kappa = 1$ in (4). To a great wave number κ now there corresponds a large support of $\tilde{a}$, namely, $\operatorname{supp}\tilde{a} = \kappa \operatorname{supp} a$. Further, instead of u^i, an entire solution to Helmholtz equation, we consider an arbitrary sufficiently smooth function $f : \mathbb{R}^n \to \mathbb{C}$. Thus our problem reads as follows: given a piecewise smooth function $a : \mathbb{R}^n \to \mathbb{C}$ with support in an open bounded set $G \subset \mathbb{R}^n$, and a smooth function $f : \mathbb{R}^n \to \mathbb{C}$, find $u : G \to \mathbb{R}^n$ satisfying the integral equation

$$u(x) = f(x) - \int_G \Phi(|x - y|)a(y)u(y)dy \qquad (x \in G)\,. \tag{6}$$

Recall that Φ is given by formula (5). Solving (6) we obtain $u(x)$ for $x \in G$; for $x \in \mathbb{R}^n \backslash G$, $u(x)$ can be obtained after that by simple integration. Notice that due to the Fredholm alternative, equation (6) remains to be uniquely solvable if it is uniquely solvable for $f(x) = u^i(x)$, i.e. if problem (1)–(3) is uniquely solvable. Now we make precise conditions on a used in this section. We assume that

$$a \in W^{2,\infty}(G \backslash \Gamma)$$

where Γ consists of a finite number of piecewise smooth compact surfaces Γ_i (for $n = 3$) or curves Γ_i (for $n = 2$) which may meet each other along manifolds of dimension $\le n - 2$. More precisely, every Γ_i satisfies the following condition (PS): there exist constants $c_0 > 0$ and $r_0 > 0$ such that, for $x \in \Gamma_i$, the piece $\Gamma_i \cap \overline{B}(x, r_0)$ of

Γ_i is representable in the form $z_n = \varphi(z')$, $z' = (z_1, \ldots, z_{n-1}) \in Z_{i,x}$ where $z_1, \ldots, z_n$ is a suitable orthogonal system of coordinates obtained from the original system $x_1, \ldots, x_n$ by tha translation of the origin into the point x and a rotation of axes; $Z_{i,x} \subset \mathbb{R}^{n-1}$ is a bounded closed region and $\varphi = \varphi_{i,x}$ is a continuous function on $Z_{i,x}$ which is continuously differentiable with $|\mathrm{grad}\varphi(z')| \leq c_0$ everywhere in $Z_{i,x}$ except possibly a manifold of dimension $\leq n-2$. The surfaces of a ball, cylinder, cone and cube are simplest examples of Γ_i satisfying (PS), together they may build more complicated configurations, e.g. two tangential balls (one in another).

Let $h > 0$ be a discretization step. For $j = (j_1, \ldots, j_n) \in \mathbb{Z}^n$, denote

$$B_{j,h} = \left\{x = (x_1, \ldots, x_n) \in \mathbb{R}^n : \ \left(j_k - \frac{1}{2}\right)h < x_k < \left(j_k + \frac{1}{2}\right)h\,, \ k = 1, \ldots, n\right\}.$$

This is a rectangular cell with the center at jh. We define the grid approximation of a as follows. We put

$$a_{j,h} = a(jh) \ \text{ if } \ B_{j,h} \cap \Gamma = \emptyset\,;$$

in particular,

$$a_{j,h} = 0 \ \text{ if } \ B_{j,h} \cap \operatorname{supp} a = \emptyset\,.$$

For $B_{j,h} \cap \Gamma \neq \emptyset$ we put

$$a_{j,h} = h^{-n} \sum_{p=1}^{q_j} a(x_{j,h}^{(p)}) \text{ meas } B_{j,h}^{(p)} \ \text{ with some } \ x_{j,h}^{(p)} \in B_{j,h}^{(p)}$$

where $B_{j,h}^{(p)}$ $(p = 1, \ldots, q_j)$ are the connectivity components of the open set $B_{j,h} \backslash \Gamma$. The measure of $B_{j,h}^{(p)}$ may be computed approximately with an accuracy $\mathcal{O}(h^{n+1})$.

Further, define

$$\Phi_{j,h} = \begin{cases} \Phi(|j|h), & 0 \neq j \in \mathbb{Z}^n, \\ 0 & , \ j = 0\,. \end{cases}$$

Take a sufficiently large $N \in \mathbb{N}$ and an open bounded set $G \in \mathbb{R}^n$ (independent of h) such that

$$\operatorname{supp} a \subset \sum_{j \in \mathbb{Z}_N^n} \overline{B}_{j,h} \subset G \tag{7}$$

where

$$\mathbb{Z}_N^n = \{j \in \mathbb{Z}^n : \ -\frac{N}{2} < j_k \leq \frac{N}{2}\,, \ k = 1, \ldots, n\}\,.$$

We approximate (6) by the discrete problem

$$u_{j,h} = f(jh) - h^n \sum_{k \in \mathbb{Z}_N^n} \Phi_{j-k,h} a_{k,h} u_{k,h} \qquad (j \in \mathbb{Z}_N^n)\,. \tag{8}$$

This is a modification of the cubature formula method examined in [7]. The modification is performed so that the discrete problem maintains the convolution structure. The following convergence result can be followed from the general result of [7].

Theorem 1 *Assume that* $\operatorname{supp} a$ *satisfies (7),* $f \in C^2(\overline{G})$ *and* $a \in W^{2,\infty}(G \backslash \Gamma)$ *with* Γ *satisfying condition (PS). Finally, asume that the homogeneous integral equation corresponding to (6) posesses only the trivial solution. Then system (8) is uniquely solvable for all sufficiently small* $h > 0$, *and*

$$\max_{j \in \mathbb{Z}_N^n} |u_{j,h} - u(jh)| \leq ch^2(1 + |\ln h|)$$

where $u \in C(\overline{G})$ *is the solution of (6) and* $u_{j,h}$ $(j \in \mathbb{Z}_N^n)$ *is the solution of system (8).*

An application of the convolution multi-matrix of system (8) to the multi-vector $\underline{a}_h \underline{u}_h$ costs $\mathcal{O}(N^n \log N)$ arithmetical operations if FFT techniques is involved. This enables to solve system (8) with the accuracy $\mathcal{O}(h^2(1 + |\ln h|)$ in $\mathcal{O}(N^n \ln N)$ arithmetical operations using two-grid iterations. For instance, putting $M \sim N^{1/3}$ for the coarse grid, 5 iterations are sufficient; the M-multisystems can be solved e.g. by Gauss elimination. There are different other strategies for the two-grid methods. We quote to [7] for numerical schemes. In Section 3.7 we present more details in the case of smooth a and trigonometric collocation as the basis of the discretization.

3 The case of a smooth a

3.1 Periodization of the problem

From now we assume that

$$\operatorname{supp} a \subset \overline{B}(0, \varrho), \quad a \in W^{\mu,2}(\mathrm{I\!R}^n), \quad f \in W^{\mu,2}_{\mathrm{loc}}(\mathrm{I\!R}^n), \quad \mu > \frac{n}{2}. \tag{9}$$

Due to the Sobolev imbedding theorem, it follows from (9) that a and f are continuous on $\mathrm{I\!R}^n$. Denote

$$G_R = \{x \in \mathrm{I\!R}^n : |x_k| < R, \ k = 1, \ldots, n\}$$

where $R \geq 2\varrho$ is a parameter. Multiplying both sides of (6) by $a(x)$ we rewrite equation (6) with respect to $a(x)u(x)$:

$$a(x)u(x) = a(x)f(x) - a(x) \int_{G_R} \Phi(|x - y|)[a(y)u(y)]dy \qquad (x \in G_R).$$

We are interested in finding of $a(x)u(x)$ for $x \in \operatorname{supp} a \subseteq \overline{B}(0, \varrho)$. For those x, only values from $\overline{B}(0, 2\varrho)$ of the function $\Phi(|x|)$ are involved; changing Φ outside this ball, the solution $a(x)u(x)$ does not change in $\overline{B}(0, \varrho)$. We exploit this observation and define a new kernel $K(x)$ which coincides with $\Phi(|x|)$ for $x \in \overline{B}(0, 2\varrho)$. The simplest possibility is to cut $\Phi(|x|)$ off at $|x| = R$:

$$K(x) = \begin{cases} \Phi(|x|), & |x| \leq R \\ 0 \quad , & x \in G_R \backslash B(0, R), \end{cases} \qquad R \geq 2\varrho. \tag{10}$$

We also consider the possibility with smooth cutting:

$$K(x) = \Phi(|x|)\psi(|x|), \qquad x \in G_R, \ R > 2\varrho, \tag{11}$$

with $\psi: \ [0, \infty) \to \mathbb{R}$ satisfying the conditions

$$\psi \in C^\infty[0,\infty), \quad \psi(r) = 1 \ \text{ for } \ 0 \le r \le 2\varrho, \psi(r) = 0 \ \text{ for } \ r \ge R. \tag{12}$$

After that we extend functions K, a and af from G_R to $\mathbb{R}^n$ as $2R$-periodic functions with respect to $x_1, \ldots, x_n$; for extensions we use the same designations. Thus we have a multiperiodic integral equation

$$v(x) = a(x)f(x) - a(x) \int_{G_R} K(x-y)v(y)dy. \tag{13}$$

It is easy to see that a unique solvability of (6) involves a unique solvability of (13). As already explained, the solutions are related by

$$v(x) = a(x)u(x) \ \text{ for } \ x \in \overline{B}(0,\varrho),$$

moreover, v is the $2R$-periodization of au restricted to G_R. Further,

$$u(x) = f(x) - \int_{B(0,\varrho)} \Phi(|x-y|)v(y)dy \ \text{ for } \ x \in \mathbb{R}^n \tag{14}$$

and in particular

$$u(x) = f(x) - \int_{G_R} K(x-y)v(y)dy \ \text{ for } \ x \in \overline{B}(0,\varrho).$$

3.2 Periodic Sobolev spaces H^λ

The trigonometric orthonormal basis of $L^2(G_R)$ is given by

$$\varphi_j(x) = (2R)^{-n/2} \exp{(i\pi j \cdot \frac{x}{R})}, \qquad j = (j_1, \ldots, j_n) \in \mathbb{Z}^n. \tag{15}$$

Introduce the Sobolev space $H^\lambda = H^\lambda(G_R)$, $\lambda \in \mathbb{R}$, which consists of $2R$-multiperiodic functions (distributions) u having the finite norm

$$||u||_\lambda = \Big(\sum_{j \in \mathbb{Z}^n} \underline{j}^{2\lambda} |\hat{u}(j)|^2 \Big)^{1/2}.$$

Here

$$\hat{u}(j) = \int_{G_R} u(x)\overline{\varphi_j(x)}dx = \langle u, \varphi_{-j} \rangle, \qquad j \in \mathbb{Z}^n,$$

are the Fourier coefficients of u, and

$$\underline{j} = \begin{cases} |j| = (j_1^2 + \ldots + j_n^2)^{1/2}, & 0 \ne j \in \mathbb{Z}^n \\ 1 & , \ j = 0. \end{cases}$$

Notice that $H^\lambda \subset W^{\lambda,2}_{\rm loc}(\mathbb{R}^n)$, thus a function $u \in H^\lambda$ with $\lambda > n/2$ is continuous. We will also use the relation

$$u, v \in H^\lambda, \quad \lambda > n/2 \;\Rightarrow\; uv \in H^\lambda, \quad \|uv\|_\lambda \leq c_\lambda \|u\|_\lambda \|v\|_\lambda\,;$$

a proof can be constructed as in [4] where somewhat different Sobolev spaces are used.

3.3 Trigonometric collocation

Recall the designation

$$\mathbb{Z}^n_N = \{j \in \mathbb{Z}^n : \; -\frac{N}{2} < j_k \leq \frac{N}{2}, \;\; k = 1, \dots, n\}\,.$$

Let $\mathcal{T}_N$ be the N^n-dimensional linear space of trigonometric polynomials of the form $v_N = \sum_{j \in \mathbb{Z}^n_N} c_j \varphi_j$, $c_j \in \mathbb{C}$. The formula

$$P_N v = \sum_{j \in \mathbb{Z}^n_N} \hat{v}(j) \varphi_j$$

defines the orthogonal projection P_N in H^λ to $\mathcal{T}_N$. Clearly,

$$\|v - P_N v\|_\lambda \leq \Big(\frac{N}{2}\Big)^{\lambda-\mu} \|v\|_\mu \;\; \text{for} \;\; \lambda \leq \mu\,, \;\; \lambda, \mu \in \mathbb{R}\,. \tag{16}$$

For $v \in H^\mu$, $\mu > \frac{n}{2}$, we define the interpolation projection $Q_N v$ claiming

$$Q_N v \in \mathcal{T}_N\,, \quad (Q_N v)(jh) = v(jh)\,, \quad j \in \mathbb{Z}^n_N\,, \;\; \text{where} \;\; h = 2R/N\,.$$

The error of the trigonometric interpolation can be estimated by (cf. (16))

$$\|v - Q_N v\|_\lambda \leq c_{\lambda,\mu} N^{\lambda-\mu} \|v\|_\mu \;\; \text{for} \;\; 0 \leq \lambda \leq \mu\,, \;\; \mu > \frac{n}{2}\,; \tag{17}$$

a proof with a characterization of the constant $c_{\lambda,\mu}$ can be constructed following [8].

We solve the equation (13) by trigonometric collocation method

$$v_N = Q_N(af) - Q_N(aKv_N) \tag{18}$$

where K is the integral operator from (13):

$$(Kv)(x) = \int_{G_R} K(x-y) v(y) dy\,.$$

Since $K(x)$ is $2R$-periodic, the eigenvalues and eigenfunctions of the convolution operator K are known to be $\hat{K}(j)$ and $\varphi_j(x)$, respectively:

$$K\varphi_j = \hat{K}(j)\varphi_j \qquad (j \in \mathbb{Z}^n)\,.$$

In the case of cutting (10), closed formulae for $\hat{K}(j)$ are presented in Section 3.8. According to those formulae,

$$|\hat{K}(j)| \leq c_R \begin{cases} |j|^{-3/2}, & n=2 \\ |j|^{-2}\ \ , & n=3 \end{cases} \qquad (j \neq 0)\,.$$

In the case of the smooth cutting (11),

$$|\hat{K}(j)| \leq c_R |j|^{-2} \quad (j \neq 0) \ \text{ for } \ n=2 \ \text{ and } \ n=3\,.$$

We present in Section 3.8 a cheep algorithm to approximate $\hat{K}(j)$, $j \in \mathbb{Z}_N^n$, in this case.

We quote to [6] for the study of the trigonometric collocation method in a more complicated but one dimensional situation.

3.4 Matrix form of the collocation method

We have two representations of a trigonometric polynomial $v_N \in \mathcal{T}_N$: (i) through its Fourier coefficients by

$$v_N(x) = \sum_{k \in \mathbb{Z}_N^n} \hat{v}_N(k) \varphi_k(x)$$

with φ_k defined in(15); (ii) through its nodal values by

$$v_N(x) = \sum_{j \in \mathbb{Z}_N^n} v_N(jh) \varphi_{N,j}(x)\,, \qquad h = \frac{2R}{N}\,,$$

with $\varphi_{N,j} \in \mathcal{T}_N$ satisfying $\varphi_{N,j}(kh) = \delta_{j,k}$ (the Kronecker symbol), $j,k \in \mathbb{Z}_N^n$. An explicit formula for $\varphi_{N,j}$ is given by

$$\varphi_{N,j}(x) = N^{-n} \sum_{k \in \mathbb{Z}_N^n} \exp\left(i\pi k \cdot \left(\frac{x}{R} - \frac{2j}{N} \right) \right), \qquad j \in \mathbb{Z}_N^n\,.$$

It is easy to change the type of representation. Having the nodal values $\underline{v}_N$ of $v_N \in \mathcal{T}_N$, its Fourier coeficients $\hat{v}_N = \mathcal{F}_N \underline{v}_N$ are given by the discrete Fourier transformation $\mathcal{F}_N$:

$$\hat{v}_N(k) = \int_{G_R} v_N(x) \varphi_{-k}(x) dx = (2R)^{n/2} N^{-n} \sum_{j \in \mathbb{Z}_N^n} v_N(jh) \exp\left\{ -i\pi k \cdot \frac{2j}{N} \right\}, \quad k \in \mathbb{Z}_N^n\,.$$

Conversely, if we have the Fourier coefficients $\hat{v}_N$ of $v_N \in \mathcal{T}_N$, then its nodal values $\underline{v}_N = \mathcal{F}_N^{-1} \hat{v}_N$ are given by the inverse discrete Fourier transformation $\mathcal{F}_N^{-1}$:

$$v_N(jh) = (2R)^{-n/2} \sum_{k \in \mathbb{Z}_N^n} \hat{v}_N(k) \exp\left\{ i\pi k \cdot \frac{2j}{N} \right\}, \qquad j \in \mathbb{Z}_N^n\,.$$

Using the transforms $\mathcal{F}_N$ and $\mathcal{F}_N^{-1}$, the collocation method (18) can be represented as

$$\underline{v}_N = (\underline{af})_N - \underline{a}_N \mathcal{F}_N^{-1} \hat{K}_N \mathcal{F}_N \underline{v}_N$$

where $\underline{a}_N$ and $(\underline{af})_N$ present the nodal values at jh, $j \in \mathbb{Z}_N^n$, of a and af, respectevely, and $\hat{K}_N$ multiplies the Fourier coefficients $\hat{v}_N(k)$ of $\hat{v}_N = \mathcal{F}_N \underline{v}_N$ by $\hat{K}(k)$, $k \in \mathbb{Z}_N^n$; the product of $\underline{a}_N$ and $\mathcal{F}_N^{-1} \hat{K} \underline{v}_N$ is to be taken pointwise at nodes. Thus, the matrix form of the collocation method (18) is given by

$$A_N \underline{v}_N = \underline{g}_N\,, \quad A_N = I_N + \underline{a}_N \mathcal{F}_N^{-1} \hat{K}_N \mathcal{F}_N\,, \quad \underline{g}_N = (\underline{af})_N\,. \tag{19}$$

An application of $\mathcal{F}_N$ or $\mathcal{F}_N^{-1}$ to a N^n-vector $\underline{v}_N$ or $\hat{v}_N$ in a usual way costs N^{2n} multiplications and additions but the FFT does this in $\mathcal{O}(N^n \log N)$ arithmetical operations. The application of diagonal operations $\hat{K}_N$ and $\underline{a}_N$ cost N^n multiplications. Thus, the application of A_N is cheap and therefore it is appropriate to solve (19) by some iteration method. We return to this question in Sections 3.6–3.7.

With respect to Fourier coefficients, the matrix form of the collocation method (18) reads as follows:

$$\hat{A}_N \hat{v}_N = \hat{g}_N\,, \quad \hat{A}_N = I_N + \mathcal{F}_N \underline{a}_N \mathcal{F}_N^{-1} \hat{K}_N\,, \quad \hat{g}_N = \mathcal{F}_N (\underline{af})_N\,.$$

3.5 Convergence of the collocation method

Lemma 1 *Assume that $a \in H^\mu$, $\mu > n/2$, and $|\hat{K}(j)| \le c|j|^{-2}$ $(j \ne 0)$. Then*

$$\|aK - Q_N aK\|_{\mathcal{L}(H^\lambda, H^\lambda)} \le c \begin{cases} N^{\lambda-\mu}, & 0 \le \lambda \le \mu\,, \ \mu \le 2\,, \\ N^{-2}\,, & 0 \le \lambda \le \mu - 2\,, \ \mu \ge 2\,, \\ N^{\lambda-\mu}, & \mu - 2 \le \lambda \le \mu\,, \ \mu \ge 2\,. \end{cases} \tag{20}$$

Proof. First notice that $K \in \mathcal{L}(H^\lambda, H^{\lambda+2})$ for any $\lambda \in \mathbb{R}$. Consider the case $\mu \ge 2$, $0 \le \lambda \le \mu - 2$. Due to (17),

$$\|aKv - Q_N(aKv)\|_\lambda \le cN^{-2}\|aKv\|_{\lambda+2} \le c'N^{-2}\|a\|_{\lambda+2}\|Kv\|_{\lambda+2} \le c''N^{-2}\|a\|_{\lambda+2}\|v\|_\lambda$$

resulting to $\|aK - Q_N aK\|_{\mathcal{L}(H^\lambda, H^\lambda)} \le cN^{-2}$. The other cases can be analysed in a similar way. □

In the case of cutting (10), $n = 2$, we have $|\hat{K}(j)| \le c|j|^{-3/2}$ $(j \ne 0)$, and instead of (20) we obtain

$$\|aK - Q_N aK\|_{\mathcal{L}(H^\lambda, H^\lambda)} \le c \begin{cases} N^{\lambda-\mu}\,, & 0 \le \lambda \le \mu\,, \ \mu \le \frac{3}{2}\,, \\ N^{-3/2}, & 0 \le \lambda \le \mu - \frac{3}{2}\,, \ \mu \ge \frac{3}{2}\,, \\ N^{\lambda-\mu}\,, & \mu - \frac{3}{2} \le \lambda \le \mu\,, \ \mu \ge \frac{3}{2}\,. \end{cases} \tag{21}$$

Theorem 2 *Assume that the functions a and f satisfy (9), and the homogeneous problem corresponding to (1)-(3), with $\kappa = 1$, $u^i = 0$, has only the trivial solution. Then equation (13) has a unique solution $v \in H^\mu$, collocation equation (18) has a unique solution $v_N \in \mathcal{T}_N$ for $N \ge N_0$, and*

$$\|v_N - v\|_\lambda \le c\|v - Q_N v\|_\lambda \le c'\|v\|_\mu N^{\lambda-\mu}, \qquad 0 \le \lambda \le \mu\,. \tag{22}$$

Proof. The bounded inverse to $I + aK$ in $\mathcal{L}(H^\lambda, H^\lambda)$ exists since $aK \in \mathcal{L}(H^\lambda, H^\lambda)$ is compact and the homogeneous integral equation corresponding to (13) has only the trivial solution. Using (20) or (21) we obtain that the inverse to $I + Q_N aK$ in $\mathcal{L}(H^\lambda, H^\lambda)$ exists for all sufficiently great N, and

$$\|(I + Q_N aK)^{-1}\|_{\mathcal{L}(H^\lambda, H^\lambda)} \le c \qquad (0 \le \lambda \le \mu\,,\;\; N \ge N_0)\,. \tag{23}$$

Error estimate (22) follows form (23) and the equality

$$(I + Q_N aK)(v_N - v) = Q_N(af) - v - Q_N aKv = Q_N v - v\,. \qquad \square$$

Thus we have an approximation $v_N \in \mathcal{T}_N$ to the $2R$-periodic extension v of au. An approximation to u outside $B(0, \varrho)$ can be defined by the discretization of (14):

$$u_N(x) = f(x) - h^n \sum_{j \in \mathbb{Z}_N^n} \Phi(|x - jh|) v_N(jh)\,, \quad h = 2R/N\,, \quad |x| > \varrho\,.$$

It can be deduced from (22) that

$$|u_N(x) - u(x)| \le c|x|^{-(n-1)/2} \|v\|_\mu N^{-\mu}, \qquad |x| \ge 2\varrho\,, \tag{24}$$

where the constant c is independent of x and N (this constant has a bad behaviour as $|x| \to \varrho$, therefore we restricted us to $|x| \ge 2\varrho$).

The following well known asymptotic formula for the solution of (6) follows from (14) and the properties of $\Phi(r)$ as $r \to \infty$ (for the behaviour of $H_0^1(r)$, see formula 9.2.3 in [1]):

$$u(x) = f(x) - \frac{e^{i|x|}}{|x|^{(n-1)/2}} u_\infty(\hat{x}) + \mathcal{O}(|x|^{-(n+1)/2})\,, \qquad |x| \to \infty\,,$$

where $\hat{x} = x/|x|$ and the far field pattern u_∞ is defined by

$$u_\infty(\hat{x}) = \gamma_n \int_{G_R} e^{-i\hat{x}\cdot y} v(y)\,dy\,, \qquad \gamma_n = \begin{cases} \dfrac{1+i}{4\sqrt{\pi}}\,, & n = 2\,, \\ \dfrac{1}{4\pi}\,, & n = 3\,. \end{cases}$$

A natural approximation to u_∞ is given by

$$u_{\infty,N}(\hat{x}) = \gamma_n h^n \sum_{j \in \mathbb{Z}_N^n} e^{-i\hat{x}\cdot jh} v_N(jh)\,, \quad \hat{x} \in S(0,1)\,.$$

Under conditions of Theorem 2,

$$\max_{\hat{x} \in S(0,1)} |u_{\infty,N}(\hat{x}) - u_\infty(\hat{x})| \le c\|v\|_\mu N^{-\mu}. \tag{25}$$

3.6 Solution of the system of the collocation method

As already mentioned, iteration methods are most natural to solve the system (19). Due to (23), for the condition number γ_N of the system, with respect to the spectral norm, we have

$$\gamma_N := \|A_N\|\,\|A_N^{-1}\| = \|I + Q_N aK\|_{\mathcal{L}(H^0,H^0)} \|(I + Q_N aK)^{-1}\|_{\mathcal{L}(H^0,H^0)} \le \gamma$$

where the constant γ is independent of N. If v_N^k denotes the kth iteration approximation by the conjugate gradient method applied to the symmetrized system

$$A_N^* A_N \underline{v}_N = A_N^* \underline{g}_N\,, \qquad A_N^* = I_N + \mathcal{F}_N^{-1} \hat{K}_N^* \mathcal{F}_N \underline{a}_n^*\,,$$

then (see e.g. [3])

$$\|v_N^k - v_N\|_0 \le c q^k \|v_N^0 - v_N\|_0\,, \qquad q = (\gamma - 1)/(\gamma + 1)\,,$$

and the accuracy $\|v_N^k - v_N\|_0 \le cN^{-\mu}$ (cf. (22)) will be achieved in $\mathcal{O}(\log N / |\log q|)$ iteration steps. Since every iteration step costs $\mathcal{O}(N^n \log N)$ arithmetical operations, the whole cost of the method is $\mathcal{O}(N^n \log^2 N)$ arithmetical operations. This amount of the work can be reduced to $\mathcal{O}(N^n \log N)$ arithmetical operations with the help of two grid iteration schemes.

3.7 Two grid iterations

Denoting

$$g_N = Q_N(af) \in \mathcal{T}_N\,, \qquad T_N = Q_N aK \in \mathcal{L}(H^\lambda, H^\lambda)\,,$$

the collocation equation (18) can be rewritten as $v_N + T_N v_N = g_N$. Take a $M \in \mathbb{N}$ of order $M \sim N^\Theta$, $0 < \Theta < 1$. The collocation equation is equivalent to $(I + T_M)^{-1}(I + T_N)v_N = (I + T_M)^{-1} g_N$, or

$$v_N = T_{M,N} v_N + g_{M,N}$$

with

$$T_{M,N} = (I + T_M)^{-1}(T_M - T_N)\,, \qquad g_{M,N} = (I + T_M)^{-1} g_N\,.$$

Under conditions of Lemma 1 and Theorem 2 we have for $0 \le \lambda \le \mu - 2$, $\mu \ge 2$, the estimate (see (20) and (23))

$$\|T_{M,N}\|_{\mathcal{L}(H^\lambda,H^\lambda)} \le cM^{-2} \le c' N^{-2\Theta}.$$

Thus, the norm of the operator $T_{M,N}$ is small, and we may apply the iterations

$$v_N^k = T_{M,N} v_N^{k-1} + g_{M,N} \qquad (k = 1, 2, \ldots) \tag{26}$$

starting e.g. from $v_N^0 = v_M = (I + T_M)^{-1} g_M$. For the exact collocation solution v_N we have $v_N = T_{M,N} v_N + g_{M,N}$ and

$$\begin{aligned} v_N^k - v_N &= T_{M,N}(v_N^{k-1} - v_N) = \ldots = T_{M,N}^k (v_N^0 - v_N)\,, \\ \|v_N^k - v_N\|_\lambda &\le \|T_{M,N}\|_{\mathcal{L}(H^\lambda,H^\lambda)}^k (\|v_N - v\|_\lambda + \|v_M - v\|_\lambda) \\ &\le c' c^k N^{-2\Theta k + \Theta(\lambda - \mu)} \|v\|_\mu \le \varepsilon N^{\lambda - \mu} \|v\|_\mu \qquad (0 \le \lambda \le \mu) \end{aligned}$$

with a small $\varepsilon > 0$ (cf. (22)) provided that $(2k+\mu-\lambda)\Theta > \mu-\lambda$. This condition is most strong for $\lambda = 0$:

$$k > \frac{1-\Theta}{2\Theta}\mu \quad \text{for fixed} \quad \Theta \in (0,1)\,,$$

or equivalently

$$\Theta > \frac{\mu}{\mu+2k} \quad \text{for fixed} \quad k \in \mathbb{N}\,.$$

So only few iterations (26) are needed to achieve the accuracy (22) by v_N^k, and this number of iterations may be taken to be independent of N. On the other hand, if we put $\Theta > \frac{\mu}{\mu+2}$, then only one iteration (26) is sufficient, i.e. asymptotically already v_N^1 achives the accuracy (22).

To present the matrix form of the two-grid iterations (26), notice that

$$(I+T_M)^{-1} = I - (I+T_M)^{-1}T_M\,.$$

Thus (26) can be written in the form where $(I-T_M)^{-1}$ is applied only to functions from $\mathcal{T}_M$:

$$v_N^k = [I-(I+T_M)^{-1}T_M][(T_M-T_N)v_N^{k-1} + g_N]\,.$$

With respect to the Fourier coefficients of v_N^k, the matrix form of the two-grid iterations (26) is as follows:

$$\begin{aligned}\hat{v}_N^k \;&=\; [I_N - \hat{P}_{N,M}\hat{A}_M^{-1}\mathcal{F}_M\underline{a}_M R_{M,N}\mathcal{F}_N^{-1}\hat{K}_N][\hat{g}_N \\ &\qquad +(\hat{P}_{N,M}\mathcal{F}_M\underline{a}_M R_{M,N} - \mathcal{F}_N\underline{a}_N)\mathcal{F}_N^{-1}\hat{K}_N\hat{v}_N^{k-1}]\,. \qquad (27)\end{aligned}$$

The designations $\hat{A}_N$, $\mathcal{F}_N$, $\mathcal{F}_N^{-1}$, $\hat{K}_N$, $\underline{a}_N$, $\hat{g}_N$ have been explained in Section 3.4; $R_{M,N}\underline{w}_N$ restricts $\underline{w}_N$ from the net $hZ_N^n = \{hj\,:\, j \in \mathbb{Z}_N^n\}$, $h = \frac{2R}{N}$, to the subnet $h'\mathbb{Z}_M^n$, $h' = \frac{2R}{M}$ (we assume that $h'/h = N/M$ is an integer); the prolongation operator $\hat{P}_{N,M}$ is defined by

$$(\hat{P}_{N,M}\hat{w}_M)(j) = \begin{cases} \hat{w}_M(j), & j \in \mathbb{Z}_M^n\,, \\ \quad 0 \quad, & j \in \mathbb{Z}_N^n \backslash \mathbb{Z}_M^n\,. \end{cases}$$

Of course, a vector $u_M = \hat{A}_M^{-1}w_M$ is computed solving the M^n-system $\hat{A}_M u_M = w_M$. This can be done e.g. by the conjugate gradient method in $\mathcal{O}(M^n\log^2 M) = \mathcal{O}(N^{\Theta n}\log^2 N)$ arithmetical operations as explained in Section 3.6. For $0 < \Theta \le 1/3$, also a direct solution of the M^n-system e.g. by the Gauss elimination holds the amount of work in $\mathcal{O}(N^n)$ arithmetical operations.

Most costful operations in (27) are $\mathcal{F}_N$ and $\mathcal{F}_N^{-1}$. During one iterations, they occur three times, plus once to compute $\hat{g}_N$. Asymptotically most cheep version of (27) is obtained putting $\Theta > \mu/(\mu+2)$. As explained, then only one iteration (26) is sufficient to achive the accuracy (22); respectively, only once we have to solve M^n-system in iteration(27), and once it should be done to compute the initial guess $\hat{v}_N^0 = \hat{v}_M = \hat{A}_M^{-1}\hat{g}_M$. The whole amount of the computational work is $\mathcal{O}(N^n\log N)$ arithmetical operations, and it is caused by 4 operations with $\mathcal{F}_N$ and $\mathcal{F}_N^{-1}$; all other operations cost $\mathcal{O}(N^n)$ or less.

Recall that this analysis is based on (20) for $0 \le \lambda \le \mu-2$, $\mu \ge 2$. It is easy to complete the analysis considering other cases in (20) and (21).

3.8 Appendix: Fourier coefficients of $K(x)$

Clearly, $(\Delta+1)\varphi_j = (1-\pi^2|j|^2/R^2)\varphi_j$. For $\pi|j| \neq R$, denoting $\lambda_j = R^2/(\pi^2|j|^2-R^2)$, with help of the Green formula we obtain

$$\begin{aligned}
\hat{K}(j) &= \int_{G_R} K(x)\varphi_{-j}(x)dx = -\lambda_j \int_{G_R} K(x)(\Delta+1)\varphi_{-j}(x)dx \\
&= -\lambda_j \lim_{\delta\to 0} \int_{B(0,R)\setminus B(0,\delta)} K(x)(\Delta+1)\varphi_{-1}(x)dx \\
&= -\lambda \lim_{\delta\to 0} \Bigg\{ \Big(\int_{S(0,R)} - \int_{S(0,\delta)} \Big) \Big(K\frac{\partial\varphi_{-j}}{\partial r} - \frac{\partial K}{\partial r}\varphi_{-j} \Big) dS \\
&\qquad + \int_{B(0.R)\setminus B(0,\delta)} ((\Delta+1)K(x))\varphi_{-j}(x)dx \Bigg\}
\end{aligned}$$

where $\frac{\partial}{\partial r} = \sum_{k=1}^n \frac{x_k}{|x|}\frac{\partial}{\partial x_k}$. According to the construction (see (10) and (11)) $K(x) = \Phi(|x|)$ on the sphere $(n = 3)$ or circle $(n = 2)$ $S(0,\delta)$. Taking ino account the asymptotics of $\Phi(r)$ and $\Phi'(r)$ as $r \to 0$, we obtain

$$\begin{aligned}
\hat{K}(j) &= \lambda_j \Bigg\{ \varphi_{-j}(0) - \int_{S(0,R)} \Big(K\frac{\partial\varphi_{-j}}{\partial r} - \frac{\partial K}{\partial r}\varphi_{-j} \Big) dS \\
&\qquad - \lim_{\delta\to 0} \int_{B(0,R)\setminus B(0,\delta)} ((\Delta+1)K(x))\varphi_{-j}(x)dx \Bigg\}. \qquad (28)
\end{aligned}$$

Cutting (10), $n = 3$. According to (10), since $(\Delta+1)K(x) = (\Delta+1)\Phi(|x|) = 0$ for $0 \neq x \in B(0,R)$, (28) reduces to

$$\hat{K}(j) = \lambda\Big\{\varphi_{-j}(0) - \Phi(R)\int_{S(0,R)} \frac{\partial\varphi_{-j}}{\partial r} dS + \Phi'(R)\int_{S(0,R)} \varphi_{-j} dS\Big\}.$$

We use the symmetry argument to evaluate

$$\begin{aligned}
\int_{S(0,R)} e^{i\pi j\cdot x/R} dS &= R^2 \int_{S(0,1)} e^{i\pi j\cdot x} dS = R^2 \int_{S(0,1)} e^{i\pi|j|x_1} dS \\
&= R^2 \int_{-1}^{1} e^{i\pi|j|x_1} 2\pi dx_1 = \frac{4R^2}{|j|}\sin(\pi|j|), \qquad j \neq 0.
\end{aligned}$$

Similarly

$$\int_{S(0,R)} \frac{\partial}{\partial r} e^{i\pi j\cdot x/R} dS = \frac{1}{R}\int_{S(0,R)} \Big(i\pi j\cdot\frac{x}{R}\Big) e^{i\pi j\cdot x/R} dS$$

$$= R \int_{S(0,1)} (i\pi \cdot x) e^{i\pi j\cdot x} dS = R \int_{S(0,1)} i\pi |j| x_1 e^{i\pi |j| x_1} dS$$

$$= Ri\pi |j| \int_{-1}^{1} x_1 e^{i\pi|j|x_1} 2\pi dx_1 = 4\pi R \cos(\pi|j|) - \frac{4R}{|j|}\sin(\pi|j|)\,, \qquad j \neq 0\,.$$

Recalling that $\varphi_{-j}(x) = (2R)^{-3/2}\exp\left(-i\pi j \cdot \frac{x}{R}\right)$ for $n = 3$, this results to

$$\begin{aligned} \hat{K}(j) &= \frac{R^2}{\pi^2|j|^2 - R^2}(2R)^{-3/2}\Big[1 - e^{iR}\Big(\cos(\pi|j|) - i\frac{R}{\pi|j|}\sin(\pi|j|)\Big)\Big]\,, \qquad j \neq 0\,, \\ \hat{K}(0) &= -(2R)^{-3/2}[1 - e^{iR}(1 - Ri)]\,. \end{aligned}$$

For $\pi|j| = R$ we obtain

$$\hat{K}(j) = -i2^{-5/2}R^{-1/2}(1 - e^{iR}R^{-1}\sin R)$$

by the L'Hospital rule or directly noticing that

$$\Phi(|x|) = \frac{1}{8\pi i}(\Delta + 1)e^{i|x|} \quad \text{for} \quad n = 3\,.$$

Clearly $|\hat{K}(j)| \leq c|j|^{-2}$ $(j \neq 0)$ in the case of cutting (10), $n = 3$.

Cutting (10), $n = 2$. Now

$$\begin{aligned} \int_{S(0,R)} e^{i\pi j\cdot x/R} ds &= R \int_{S(0,1)} e^{i\pi j\cdot x} ds = R \int_{S(0,1)} e^{i\pi|j|x_1} ds \\ &= 2R \int_{-1}^{1} e^{i\pi|j|x_1}(1 - x_1^2)^{-1/2} ds_1 = 4R \int_0^1 \cos(\pi|j|x_1)(1 - x_1^2)^{-1/2} dx_1 \\ &= 2\pi R J_0(\pi|j|) \end{aligned}$$

and similarly

$$\int_{S(0,R)} \frac{\partial}{\partial r} e^{i\pi j\cdot x/R} ds = -2\pi^2|j|J_1(\pi|j|)$$

(see [1], formulae 9.1.20 and 9.1.28 for the Bessel fubctions J_0 and J_1). This results to

$$\begin{aligned} \hat{K}(j) &= \frac{R^2}{\pi^2|j|^2 - R^2}(2R)^{-1}\Big\{1 + \frac{1}{2}i\pi\Big[\pi|j|J_1(\pi|j|)H_0^1(R) - RJ_0(\pi|j|)H_1^1(R)\Big]\Big\} \\ &\qquad\qquad \text{for} \quad \pi|j| \neq R\,, \qquad j \neq 0\,, \\ \hat{K}(0) &= -(2R)^{-1} - \pi\Phi'(R) = -(2R)^{-1} + \frac{\pi i}{4}H_1^{(1)}(R)\,, \\ \hat{K}(j) &= \frac{1}{8}\pi Ri\Big[J_0(R)H_0^{(1)}(R) + J_1(R)H_1^{(1)}(R)\Big] \quad \text{for} \quad \pi|j| = R\,. \end{aligned}$$

Since $J_\nu(r) \sim \sqrt{2/(\pi r)}\cos(r - \frac{1}{2}\nu\pi - \frac{1}{4}\pi)$ as $r \to \infty$ (see [1], formula 9.2.1), we have $|\hat{K}(j)| \leq c|j|^{-3/2}$ $(j \neq 0)$ in the case of cutting (10), $n = 2$.

Cutting (11), $n = 2$ or $n = 3$. Using the soft cutting (11) we obtain from (28)

$$\hat{K}(j) = \lambda_j \Big\{ (2R)^{-n/2} - \int\limits_{G_R} (2\nabla\Phi \cdot \nabla\psi + \Phi\Delta\psi)\varphi_{-j} dx \Big\} = \lambda_j \{ (2R)^{-n/2} - \hat{\chi}(j) \}$$

where the function

$$\chi(x) := 2\nabla\Phi(|x|) \cdot \nabla\psi(|x|) + \Phi(|x|)\Delta\psi(|x|) = 2\Phi'(r)\psi'(r) + \Phi(r)[\psi''(r) + 2r^{-1}\psi'(r)]$$

is C^∞-smooth and supported on the annulus $2\varrho \le r \le R$ (see (12). Therefore $|\hat{\chi}(j)| \le c_p |j|^{-p}$ $(0 \ne j \in \mathbb{Z}^n)$ with any $p > 0$, and $|\hat{K}(j)| \le c|\lambda_j| \le c'|j|^{-2}$ $(j \ne 0)$. Approximating χ by $Q_M\chi$, $M \sim N^\Theta$, $0 < \Theta \le 1$, we have

$$\max_{x \in G_R} |\chi(x) - (Q_M\chi)(x)| \le c\|\chi - Q_M\chi\|_2 \le c_p M^{-p} \|\chi\|_{p+2}$$

with any $p > 0$. The computation of $(\widehat{Q_M\chi})(j)$, $j \in \mathbb{Z}^n_M$, from grid values of χ by FFT costs $\mathcal{O}(M^n \log M)$ arithmetical operations. Thus, we have a cheep way to compute the approximations

$$\begin{aligned} \hat{K}_N(j) &= \frac{R^2}{\pi^2|j|^2 - R^2} \Big\{ (2R)^{-n/2} - (\widehat{Q_M\chi})(j) \Big\} \quad \text{for } j \in \mathbb{Z}^n_M, \\ \hat{K}_N(j) &= \frac{R^2}{\pi^2|j|^2 - R^2} (2R)^{-n/2} \quad \text{for } \ j \in \mathbb{Z}^n_N \backslash \mathbb{Z}^n_M \end{aligned}$$

to $\hat{K}(j)$ of a high accuracy:

$$\max_{j \in \mathbb{Z}^n_N} |\hat{K}_N(j) - \hat{K}(j) \le c_p N^{-\Theta p} \|\chi\|_{p+2} \ \text{ with any } \ p > 0\,. \tag{29}$$

There is also a possibility for an exact expression of $\hat{\chi}(j)$ through integrals on $(2\varrho, R)$ from some smooth functions containing the multipliers $\psi'(r)$ and $\psi''(r)$.

Let us briefly discuss also the construction of cutting function ψ satisfying (12). Take a function $\varphi \in C^\infty[0, \infty)$ such that $\varphi^{(k)}(0) = 0$ for all $k = 0, 1, 2, \ldots$, e.g. $\varphi(s) = e^{-\delta/s}$, $\delta > 0$. Then

$$\psi(r) := \begin{cases} 1 & , \ 0 \le r \le 2\varrho \\ c_0^{-1} \int_r^R \varphi(s - 2\varrho)\varphi(R - s) ds, & 2\varrho \le r \le R \\ 0 & , \ r \ge R \end{cases}$$

with

$$c_0 = \int_{2\varrho}^R \varphi(s - 2\varrho)\varphi(R - s) ds$$

satisfies (12). A fortune is that we need only derivatives $\psi'(r)$ and $\psi''(r)$, not $\psi(r)$ itself, and the derivatives of ψ are available from the formula. The only integral defining c_0 can be approximated with a high accuracy by the trapezoidal rule since the integrand and all its derivatives vanish at the end points 2ϱ and R. If we put $\varphi(s) = s^m$ we have $c_0 = \frac{(m!)^2}{(2m)!}(R - 2\varrho)^{2m-1}$ and $\psi \in C^m[0, \infty)$. With m sufficiently large, also this cutting function ψ is suitable for our purposes.

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