GENERALIZED COMBINED FIELD INTEGRAL EQUATIONS FOR THE ITERATIVE SOLUTION OF THE HELMHOLTZ EQUATION IN THREE DIMENSIONS

XAVIER ANTOINE* AND MARION DARBAS†

Abstract. This paper addresses the derivation of new second-kind Fredholm combined field integral equations for the Krylov iterative solution of acoustic scattering problems. These integral equations need the introduction of suitable tangential square-root operators to regularize the formulations. Existence and uniqueness occur for these formulations. They can be interpreted as generalizations of the well-known Brakhage-Werner [A. Brakhage and P. Werner, *Über das Dirichletsche aussenraumproblem für die Helmholtzsche schwingungsgleichung*, Arch. Math. **16** (1965), pp. 325-329] and Combined Field Integral Equations (CFIE) [R.F. Harrington and J.R. Mautz, *H-field, E-field and combined field solution for conducting bodies of revolution*, Arch. Elektron. Übertragungstech (AEÜ), 32 (4) (1978), pp. 157-164]. Finally, two- and three-dimensional numerical experiments are performed to test their efficiency.

Key words. Acoustic and electromagnetic scattering, Helmholtz equation, second-kind Fredholm integral equation, Krylov iterative solution

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1. Introduction. Integral equations are widely used in modern acoustic and electromagnetic scattering codes for solving large scale problems in the high-frequency regime [22]. These developments have been strongly influenced by the introduction of fast solvers as for instance the Fast Multipole Method (FMM) of Rokhlin [22, 42] or other recent high-order solvers [10, 11]. The FMM leads to a computational cost of a matrix-vector product of the order of $\mathcal{O}(n \log n)$ instead of $\mathcal{O}(n^2)$ for a dense complex matrix of size n. Generally, a preconditioner is associated to this resolution to get a good convergence rate of the iterative solver and to obtain lower computational times. Numerous works have been devoted to this problem. Maybe the most widely developed approach is based on algebraic solvers like for instance the SPAI preconditioners [15, 16, 18, 20], the methods based on the operators splitting [2, 17] or the wavelet-based preconditioners [19, 29]. The ill-conditioning of the linear system to solve is often linked to the fact that the underlying integral equation is a first-kind Fredholm equation but also to the physics through the coupling of non-local modes [6, 22, 23]. This is for instance the case of the Electric Field Integral Equations (EFIE) [22], the Brakhage-Werner [9, 12, 26, 36] (also sometimes called Burton-Miller [2, 12]) integral equations and the Combined Field Integral Equation (CFIE) of Mautz and Harrington [30] for a Neumann boundary condition. Second-kind integral equations have generally a much better convergence rate when they are solved e.g. by the GMRES [43, 44]. Superlinear convergence phenomenon then occurs [13, 35, 41]. The scattering problem is not elliptic and leads to highly indefinite linear systems of equations. Therefore, algebraic solvers designed for this class of operators should not naturally yield *a priori* good convergence properties for solving integral equations in diffraction. This suggests that the physical nature of the problems and the mathematical structure of the underlying Helmholtz equation should be more appropriately taken into account in the construction of an efficient preconditioner.

*Laboratoire de Mathématiques pour l'Industrie et la Physique, CNRS UMR 5640, Université Paul Sabatier, 118 Route de Narbonne, 31062 Toulouse Cedex 4, France. (antoine@mip.ups-tlse.fr).

†Département de Génie Mathématique, INSA, MIP UMR-5640, Complexe Scientifique de Rangueil, 31077, Toulouse cedex 4, France. (darbas@gmm.insa-tlse.fr).

Such a tentative has been recently developed by Christiansen and Nédélec [24, 25] who have used the Caldèron relations [45] for designing an analytical preconditioner for the EFIE for the scattering problem by an open surface. Another possibility based on the construction of a local preconditioner has also been presented in [6]. However for a closed surface, the EFIE suffers from the presence of internal resonant modes and is hence ill-posed [26]. For these reasons, Brakhage-Werner and combined field integral equations are generally preferred [22, 26].

The aim of this paper is to propose some second-kind Fredholm combined field integral equations for the three-dimensional acoustic scattering problem by a closed surface. These new formulations can be seen as a generalization of both the Brakhage-Werner and Combined Field Integral Equations [7, 38]. Their construction is based on the integration of efficient pseudodifferential operators to regularize the trace of the single-layer potential or the normal derivative trace of the double-layer potential according to the scattering problem to solve. These regularizing operators expressed as square-root tangential operators are derived from ideas arising in Beam Propagation Methods [31, 39, 46]. They also fall into the general framework of On-Surface Radiation Conditions introduced in the middle of the eighties by Kriegsmann *et al.* [37] and studied by several authors [3, 4, 8, 14, 32, 33, 34]. Like the Brakhage-Werner integral equations and the CFIE and unlike the EFIE, these integral equations are uniquely solvable at any frequency for a closed surface [26]. This is an important property for the applications for instance in inverse scattering problems [27]. These new alternative integral equations are constructed as second-kind Fredholm integral equations and are therefore characterized by an excellent eigenvalue clustering. This central property leads to a superlinear convergence of the GMRES [13, 35, 41].

The plan of the paper is the following. In section 2, we present the general problem setting and some basic results about the integral equation representations for the Helmholtz equation. In section 3, we define the general process for designing some generalizations of the Brakhage-Werner integral equations based on the use of the Dirichlet-Neumann (DN) and Neumann-Dirichlet (ND) maps. This construction follows the ideas developed in [7] and is presented as a generalization of the Brakhage-Werner integral equations. In section 4, we build an efficient and simple approximation of both the DN and ND operators by using some similar techniques as in the Beam Propagation Methods [39, 31] working in a generalized coordinates system. Section 5 is devoted to the well-posedness of the new integral equations at any frequency. In section 6, we calculate the eigenvalues of the new operators and numerically show that the new integral equations have an excellent eigenvalue clustering even for high-frequencies for the model problem of the scattering of a plane wave by a sphere. In section 7, we extend our ideas to a generalization of the usual CFIE of Harrington and Mautz [30]. We develop several aspects linked to the implementation of the new integrals in a Krylov iterative solver in the 8th section. An essential aspect is that the approximations of the DN and ND operators are computed by paraxialization techniques [40]. In section 9, we perform some numerical experiments to show that the new integral equations have some excellent convergence rates to solve two- and three-dimensional scattering problems.

2. Integral representations for acoustic scattering. Let us consider a smooth closed bounded set $\Omega^- \subset \mathbb{R}^d$ $(d = 2, 3)$ whose boundary $\Gamma = \partial\Omega^-$ is a $(d-1)$-dimensional regular compact manifold. Let us define $\Omega^+ = \mathbb{R}^d \setminus \overline{\Omega^-}$ as the associated exterior domain of propagation. We consider an incident time-harmonic acoustic wave u^{inc} defined by the wavenumber $k = 2\pi/\lambda$, setting λ as the wavelength of the incident field. The time-dependence is $e^{-i\omega t}$, denoting by ω the frequency of the signal. Then, the diffraction boundary value problem can be written as

$$\left\{\begin{array}{l} \text{Find } u^+ \in H^1_{\mathrm{loc}}(\overline{\Omega^+}) \text{ such that} \\ \Delta u^+ + k^2 u^+ = 0, \quad \text{in } \mathcal{D}'(\Omega^+), \\ \gamma_j^+ u^+ = g, \quad \text{in } H^{1/2-j}(\Gamma), \qquad \text{for } j = 0 \text{ or } 1, \\ \lim\limits_{|x|\to+\infty} |x|^{(d-1)/2} \left(\nabla u^+ \cdot \dfrac{x}{|x|} - iku^+\right) = 0, \end{array}\right. \tag{2.1}$$

where $H^1_{\mathrm{loc}}(\overline{\Omega^+})$ designates the Fréchet space

$$H^1_{\mathrm{loc}}(\overline{\Omega^+}) := \left\{ v \in \mathcal{D}'(\Omega^+)/\psi v \in H^1(\Omega^+), \forall \psi \in \mathcal{D}(\mathbb{R}^d) \right\}.$$

The first equation of system (2.1) is the so-called Helmholtz equation. We restrict our study here to a Dirichlet (for $g = -\gamma_0^+ u^{\mathrm{inc}}$) or a Neumann (for $g = -\gamma_1^+ u^{\mathrm{inc}}$) boundary condition, where γ_j^+ is the exterior trace of order j (see (2.4)). For acoustic radiation problems, these boundary conditions respectively correspond to the scattering problem by a sound-soft or a sound-hard body. Finally, the well-known Sommerfeld radiation condition at infinity is imposed to ensure the uniqueness of the solution to the boundary value problem (2.1).

We can associate to (2.1) the following interior boundary value problem

$$\left\{\begin{array}{l} \text{Find } u^- \in H^1(\Omega^-) \text{ such that} \\ \Delta u^- + k^2 u^- = 0, \quad \text{in } \mathcal{D}'(\Omega^-), \\ \gamma_j^- u^- = g, \quad \text{in } H^{1/2-j}(\Gamma), \qquad \text{for } j = 0 \text{ or } 1. \end{array}\right. \tag{2.2}$$

Let us introduce the Sobolev spaces

$$\begin{aligned} H^1_-(\Delta) &:= H^1(\Delta, \overline{\Omega^-}) := \left\{ u \in H^1(\overline{\Omega^-}); \Delta u \in L^2(\overline{\Omega^-}) \right\}, \\ H^1_+(\Delta) &:= H^1_{\mathrm{loc}}(\Delta, \overline{\Omega^+}) := \left\{ u \in H^1_{\mathrm{loc}}(\overline{\Omega^+}); \Delta u \in L^2(\overline{\Omega^+}) \right\}. \end{aligned} \tag{2.3}$$

Then, for $u^\pm \in H^1_\pm(\Delta)$, the exterior $(+)$ and interior $(-)$ trace operators of order j ($j = 0$ or 1) can be both defined

$$\begin{aligned} \gamma_j^\pm : H^1_\pm(\Delta) &\to H^{1/2-j}(\Gamma) \\ u^\pm &\mapsto \gamma_j^\pm u^\pm = \partial^j_{\mathbf{n}} u^\pm_{|\Gamma}. \end{aligned} \tag{2.4}$$

Vector $\mathbf{n}$ is the outwardly directed unit vector to Ω^-.

One of the main difficulties arising in the solution of an exterior boundary value problem is related to the unboundedness of the domain Ω^+. Among the most widely used solutions are the integral equation formulations [22, 26]. This technique consists in rewriting the initial problem (2.1) equivalently as an integral equation set on the finite surface Γ. The first step is based on the use of the integral representation of the exterior field u^+ as the superposition of the single- and double-layer potentials L and M as follows

$$u^\pm = -M\gamma_0^\pm u^\pm - L\gamma_1^\pm u^\pm.$$

Therefore, the Cauchy data $(\gamma_0^+ u^+, \gamma_1^+ u^+)$ become the new unknowns. The integral operators L and M are respectively given by

$$\begin{aligned} Lp(x) &= \int_\Gamma G(x,y)p(y)d\Gamma(y), \quad \forall x \in \Omega^- \cup \Gamma \cup \Omega^+, \\ M\phi(x) &= -\int_\Gamma \partial_{\mathbf{n}(y)} G(x,y)\phi(y)d\Gamma(y), \quad \forall x \in \Omega^- \cup \Gamma \cup \Omega^+, \end{aligned} \tag{2.5}$$

for two well-defined densities p and ϕ. Function G stands for the Green's kernel associated to the Helmholtz operator $(\Delta + k^2)$

$$G(x,y) = \frac{i}{4}\left(\frac{k}{2\pi|x-y|}\right)^{(d-2)/2} H^{(1)}_{(d-2)/2}(k|x-y|), \quad x \neq y, \tag{2.6}$$

where $H_t^{(1)}$ is the Hankel function of the first kind and order t. These two operators can be understood in the sense of the Lebesgue integral and map from $H^{-1/2}(\Gamma)$ onto $H^{1/2}(\Gamma)$.

Since our goal is to write an integral equation on Γ for using the boundary condition and to next determine the remaining unknown, we have to express the first two traces of $u^{\pm}$.

PROPOSITION 2.1. *Under the previous notations, the first two traces of $u^{\pm} \in H^1_{\pm}(\Delta)$ are related by the integral representations*

$$\gamma_0^{\pm} u^{\pm} = (\pm \frac{I}{2} - M)\gamma_0^{\pm} u^{\pm} - L\gamma_1^{\pm} u^{\pm}, \quad \textit{in } H^{1/2}(\Gamma), \tag{2.7}$$

and

$$\gamma_1^{\pm} u^{\pm} = (\pm \frac{I}{2} - N)\gamma_1^{\pm} u^{\pm} - D\gamma_0^{\pm} u^{\pm}, \quad \textit{in } H^{-1/2}(\Gamma),$$

where I is the identity operator.

The operators N and D are respectively the normal derivatives of the single- and double-layer potentials and are given by

$$\begin{aligned} Np(x) &= \partial_{\mathbf{n}(x)} \int_\Gamma G(x,y)p(y)d\Gamma(y) = -M^t p, \quad \forall x \in \Gamma, \\ D\phi(x) &= -\partial_{\mathbf{n}(x)} \int_\Gamma \partial_{\mathbf{n}(y)} G(x,y)\phi(y)d\Gamma(y), \quad \forall x \in \Gamma. \end{aligned} \tag{2.8}$$

In the above relations, A^t designates the transposed operator of an operator A. The hypersingular integral operator D maps from $H^{1/2}(\Gamma)$ onto $H^{-1/2}(\Gamma)$.

3. Generalized Brakhage-Werner integral formulations. Different ways of designing integral equations for solving (2.1) exist. We propose here to construct some new second-kind Fredholm integral equations well-suited for the iterative solution by a Krylov solver. Among the most widely used formulations are the Brakhage-Werner integral formulations. These formulations are based on the representation of the scattered field as a linear combination of the single- and double-layer potentials applied to some non-physical densities. We propose here a general background for generalizing such formulations.

Firstly, let us consider the case of a Dirichlet boundary condition and let us start with the exterior integral representation (2.7)

$$(\frac{I}{2} - M)\gamma_0^+ u^+ - L(\gamma_1^+ u^+) = g, \quad \text{in } H^{1/2}(\Gamma). \tag{3.1}$$

A well-known result is that the integral equation resulting from replacing $\gamma_0^+ u^+$ by g and solved according to the normal derivative trace is ill-posed. The presence of resonance eigenvalues associated to the interior boundary value problem leads to the non-uniqueness of the solution to the integral equation. For this reason, formulations based on combined single- and double-layer potentials are rather preferred like for instance the ones proposed by Brakhage-Werner (BW) and Burton-Miller [26]. More precisely, their approach consists in determining an unknown density ψ solution to the BW equation

$$(\frac{I}{2} - M - \eta L)\psi = g, \text{ in } H^{1/2}(\Gamma). \tag{3.2}$$

These formulations are well-posed for any wavenumber k as long as the coupling parameter η has a positive imaginary part [26]. Moreover, a numerical study due to Kress [36] shows that an "almost optimal" coupling parameter η to yield a minimal condition number of the operator defining (3.2) is $\eta = ik$. These formulations can be generalized as follows [7]. Let us assume that the exact Dirichlet-Neumann (DN) map $\mathbf{\Lambda}^{\text{ex}}$ given by [5]

$$\begin{array}{llll} \mathbf{\Lambda}^{\text{ex}}: & H^{1/2}(\Gamma) & \rightarrow & H^{-1/2}(\Gamma) \\ & \gamma_0^+ u^+ & \mapsto & \gamma_1^+ u^+ = \mathbf{\Lambda}^{\text{ex}} \gamma_0^+ u^+, \end{array} \tag{3.3}$$

is known. Then, the exterior normal derivative trace can be directly computed from $\gamma_1^+ u^+ = \mathbf{\Lambda}^{\text{ex}} g$. Moreover, from (3.1) and (3.3) the following identity holds

$$\frac{I}{2} - M - L\mathbf{\Lambda}^{\text{ex}} = I.$$

Nevertheless, one generally cannot compute the DN operator for a general surface. The idea proposed in [7] consists in considering some suitable analytic approximations of the DN operator. Essentially, we consider an operator $\widetilde{\mathbf{\Lambda}}$ approximating the exact operator $\mathbf{\Lambda}^{\text{ex}}$ and we solve the integral equation for an unknown density ψ

$$B_D \psi = g \quad \text{in } H^{1/2}(\Gamma), \tag{3.4}$$

setting

$$B_D = (\frac{I}{2} - M) - L\widetilde{\mathbf{\Lambda}}. \tag{3.5}$$

A suitable choice of $\widetilde{\mathbf{\Lambda}}$ leads to a second-kind Fredholm integral operator well-suited for a Krylov solution. Both the normal derivative and the far-field pattern can be reconstructed from ψ using proposition 2.1. Moreover, choosing $\widetilde{\mathbf{\Lambda}} = ik$ (Sommerfeld radiation condition) yields the parameter of Kress [7]. Therefore, this approach can be seen as a generalization of the one proposed by Brakhage and Werner.

For a Neumann boundary condition, the starting point is based on the following integral formulation

$$(\frac{I}{2} - N)\gamma_1^+ u^+ - D\gamma_0^+ u^+ = g, \quad \text{in} \quad H^{-1/2}(\Gamma). \tag{3.6}$$

This equation suffers from spurious internal resonances if the normal derivative trace is replaced by g and the equation is solved according to the exterior trace $\gamma_0^+ u^+$. To construct a well-posed equation, let us make the assumption that a suitable approximation $\widetilde{\mathbf{V}}$ of the exact Neumann-Dirichlet (ND) operator $\mathbf{V}^{\text{ex}}$ can be derived. Then, one solves the following equation

$$B_N \varphi = g, \text{ in } H^{-1/2}(\Gamma), \tag{3.7}$$

with

$$B_N = (\frac{I}{2} - N) - D\widetilde{\mathbf{V}}. \tag{3.8}$$

The exterior trace of the solution can be computed by the representations (2.7) from φ and the far-field pattern can be estimated. Considering the lowest order approximation $\widetilde{\mathbf{V}} = -i/k$ (Sommerfeld radiation condition) gives the usual Brakhage-Werner integral equation with the parameter of Kress. In the sequel, equations (3.4)-(3.5) and (3.7)-(3.8) are referred to as generalized Brakhage-Werner integral equations for respectively the Dirichlet and Neumann boundary conditions.

4. An approximation of the DN and ND operators by the BPM. During the construction of the integral operators B_D and B_N, we have seen that an approximation of the DN and ND pseudodifferential operators must be derived. We propose here to follow some ideas inspired from the techniques of Beam Propagation Methods (BPM) usually employed in guided optics or underwater acoustic wave propagation to construct such approximations.

Since the boundary Γ is a compact manifold, we can describe the surface by a collection of coordinates charts. To this end, let us consider a point x of Γ. Let δ be a positive real parameter. A neighborhood $\mathcal{U}_\delta$ of Γ is given by

$$\mathcal{U}_\delta = \{x \in \mathbb{R}^d; \mathrm{dist}(x, \Gamma) < \delta\},$$

where $\mathrm{dist}(x, \Gamma)$ designates the distance of a point x to Γ. Then, for a sufficiently small value of δ, it can be proved that for any $x \in \mathcal{U}_\delta$, there exists a unique p in Γ such that: $|p - x| = \delta$. The point p is the orthogonal projection of x onto Γ. The outwardly unitary vector $\mathbf{n}$ to Γ can be locally extended to $\mathcal{U}_\delta$. Therefore, we get a natural parametrization of $\mathcal{U}_\delta$ given by

$$\mathcal{U}_\delta = \{x = p + r\mathbf{n}(p); -\delta < r < \delta, p \in \Gamma\}.$$

More precisely, for δ small enough, the map $(p, r) \mapsto x = p + r\mathbf{n}(p)$ defines a $\mathcal{C}^\infty$ diffeomorphism between $\Gamma \times (-\delta, \delta)$ and $\mathcal{U}_\delta$. For r in the interval $]-\delta, \delta[$, the parallel surface Γ_r to Γ can be described as $\Gamma_r = \{x \in \mathbb{R}^d; x = p + r\mathbf{n}(p)\}$. The unitary normal vector to Γ_r at a point x can be defined by the extension of $\mathbf{n}(x)$ and $\Gamma_0 = \Gamma$. Let us consider a local chart $(\mathcal{V}, \Psi)$ of Γ: $\Psi : \mathcal{V} \to \Gamma$. Each point p of $\Psi(\mathcal{V})$ is described by $p = \Psi(s)$. We can define the normal vector to Γ using the following rule. The chart $(\mathcal{V}, \Psi)$ gives rise to a basis $(\boldsymbol{\tau}_1, \boldsymbol{\tau}_2)$ of the tangent plane $T_p(\Gamma)$ given by: $\boldsymbol{\tau}_j = \partial_{s_j}\Psi$, for $j = 1, 2$, and s_j being the coordinates of s. We assume that the chart is compatible with the orientation of $\mathbf{n}$, i.e.

$$\mathbf{n}(p) = \frac{\boldsymbol{\tau}_1 \wedge \boldsymbol{\tau}_2}{|\boldsymbol{\tau}_1 \wedge \boldsymbol{\tau}_2|},$$

where $\mathbf{a} \wedge \mathbf{b}$ stands for the usual inner product of two vectors $\mathbf{a}$ and $\mathbf{b}$ in $\mathbb{C}^d$. From now on, we make the following choice of local chart. We choose $(\mathcal{V}, \Psi)$ such that the coordinates system (r, s) is orthonormal (i.e. $(\boldsymbol{\tau}_1, \boldsymbol{\tau}_2)$ is an orthonormal basis of the tangent plane) and such that $\boldsymbol{\tau}_j$ is an eigenvector of the curvature tensor. Then, it can be shown (see for instance [5]) that in this principal basis, we can rewrite the Helmholtz equation as

$$\partial_r^2 u + 2\mathcal{H}_r u + \frac{1}{h_1 h_2}(\partial_{s_1}(\frac{h_2}{h_1}\partial_{s_1} u) + \partial_{s_2}(\frac{h_1}{h_2}\partial_{s_2} u)) + k^2 u = 0, \quad \text{on } \Gamma_r. \tag{4.1}$$

Hereabove, we have denoted by h_j the parameter $h_j(r,s) = 1 + \kappa_j r$, for $j = 1, 2$, where the functions κ_j designate the principal curvatures of the surface. The mean curvature $\mathcal{H}_r$ is given by $\mathcal{H}_r = h_1^{-1} h_2^{-1} \partial_r (h_1 h_2)/2$.

Since we assume that we have a time dependence according to $e^{-i\omega t}$, then the Beam Propagation Method (BPM) gives that the solution to (4.1) can be approximated by the square-root operator

$$\varphi = i\sqrt{\frac{1}{h_1 h_2}(\partial_{s_1}(\frac{h_2}{h_1}\partial_{s_1}) + \partial_{s_2}(\frac{h_1}{h_2}\partial_{s_2})) + k^2}\,\psi, \quad \text{on } \Gamma_r.$$

Taking the value of this expression for $r = 0$ yields the following approximation of the DN map on Γ through the square-root surfacic operator

$$\varphi = ik\sqrt{1 + \frac{\Delta_\Gamma}{k^2}}\psi, \quad \text{on } \Gamma,$$

denoting by (ψ, φ) an approximation of the exact Cauchy data $(\gamma_0^+ u, \gamma_1^+ u)$. The square-root $\sqrt{z}$ of a complex number z designates the classical complex square-root with branch-cut along the negative real axis. The operator Δ_Γ is the usual Laplace-Beltrami operator over the surface Γ. Since Γ is a compact manifold, there exists an orthonormal basis $(\phi_j)_{j\in\mathbb{N}}$ of eigenvectors of Δ_Γ associated to the non-negative real eigenvalues $(\mu_j)_{j\in\mathbb{N}}$ and satisfying the eigenvalue problem

$$-\Delta_\Gamma \phi = \mu\phi.$$

Then the square-root operator $\mathbf{\Lambda}$ given by

$$\mathbf{\Lambda} = ik\sqrt{1 + \frac{\Delta_\Gamma}{k^2}},$$

is defined by the spectral decomposition

$$\mathbf{\Lambda}\psi = ik\sum_{j=1}^{+\infty}\sqrt{1 - \frac{\mu_j}{k^2}}\psi_j\phi_j, \quad \text{with } \psi = \sum_{j=1}^{+\infty}\psi_j\phi_j.$$

The modes j such that $\mu_j < k^2$ correspond to the propagative modes while the ones given for $\mu_j > k^2$ are linked to the evanescent modes. For scattering problems, a transition region corresponding to modes such that $\mu_j \approx k^2$ gives the grazing modes. It can be shown [8, 14] that the artificial singularity of the square-root operator does not yield a satisfactory representation of these modes. The transition from the propagative modes to the evanescent ones should be *a priori* smooth. To approximately model this behaviour, we use following [8] a regularization of $\mathbf{\Lambda}$ introducing a small local damping parameter $\varepsilon > 0$ in the transition region. More precisely, we use the following approximation of the DN operator

$$\varphi = \mathbf{\Lambda}_\varepsilon \psi \tag{4.2}$$

with

$$\mathbf{\Lambda}_\varepsilon = ik\sqrt{1 + \frac{\Delta_\Gamma}{k_\varepsilon^2}}, \tag{4.3}$$

setting $k_\varepsilon = k + i\varepsilon$. The following estimation of ε is derived in the two-dimensional case in the OSRC context [8]: $\varepsilon = 0.4k^{1/3}\kappa^{2/3}$, denoting by κ the local curvature of Γ. The formal extension to the three-dimensional case would be $\varepsilon = 0.4k^{1/3}2^{2/3}\mathcal{H}^{2/3}$, where $\mathcal{H}$ is the mean curvature of the surface Γ. However, for the sake of simplicity and from some numerical studies, it appears that we can take a constant value of ε. More precisely, a good choice of this parameter is: $\varepsilon = 0.4k^{1/3}2^{2/3}R^{-2/3}$, where R is the radius of the smallest sphere containing the scatterer.

Concerning the approximation of the ND operator, we naturally choose the following one

$$\psi = \mathbf{V}_\varepsilon \varphi \tag{4.4}$$

setting

$$\mathbf{V}_\varepsilon = \frac{1}{ik}(1 + \frac{\Delta_\Gamma}{k_\varepsilon^2})^{-1/2}. \tag{4.5}$$

5. Solvability of the generalized BW integral equations. The classical Brakhage-Werner integral equations have been constructed to be uniquely solvable. We propose here to prove that this is also the case for the generalizations of these integral formulations with the regularized square-root operator.

5.1. A preliminary result. Before giving the proof, we state a preliminary result concerning the computation of the principal symbol of the single-layer potential L and normal derivative of the double-layer potential D.

LEMMA 5.1. *Let L and D be respectively the single-layer and normal derivative trace of the double-layer potentials defined by the expressions (2.5) and (2.8). Let ξ be the dual variable of x by Fourier transform for x restricted to Γ. Then, the principal symbols of L and D, denoted by $\sigma_p(L)$ and $\sigma_p(D)$, are given by*

$$\sigma_p(L) = \frac{i}{2\sqrt{k^2 - |\xi|^2}} \quad \textit{and} \quad \sigma_p(D) = \frac{\sqrt{k^2 - |\xi|^2}}{2i}. \tag{5.1}$$

Proof. We do not detail the proof. Essentially, the arguments follow the ones given e.g. in [21] (pp. 88-93) for the Laplace operator. The main difference is that the presence of the wavenumber in the definition of the Helmholtz operator leads to incorporate k in the calculation of the principal symbol. □

5.2. The sound-soft scattering problem. The generalized Brakhage-Werner integral equation for the Dirichlet boundary condition is given by

$$B_{D,\varepsilon}\psi = g, \text{ in } H^{1/2}(\Gamma), \tag{5.2}$$

where the integral operator $B_{D,\varepsilon}$ is defined by $B_{D,\varepsilon} = (I/2 - M) - L\mathbf{\Lambda}_\varepsilon$. The operators M and L are given by the representations (2.5). The square-root operator $\mathbf{\Lambda}_\varepsilon$ is expressed following (4.3). Then, the following result holds.

PROPOSITION 5.2. *The integral equation (5.2) is uniquely solvable for any frequency $k > 0$ and damping parameter $\varepsilon > 0$.*

Proof. The first point consists in stating that the operator $B_{D,\varepsilon}$ can be written as $aI + K$, where $a \neq 0$ is a constant and K a compact operator from $H^{1/2}(\Gamma)$. From

Lemma 5.1 and the expression (4.3) of the square-root operator $\mathbf{\Lambda}_\varepsilon$, we straightforwardly have the respective principal symbol of these operators

$$\sigma_p(L) = \frac{-1}{2|\xi|\sqrt{1-k^2/|\xi|^2}} \text{ and } \sigma_p(\mathbf{\Lambda}_\varepsilon) = \frac{k}{k_\varepsilon}|\xi|\sqrt{1-\frac{k_\varepsilon^2}{|\xi|^2}}.$$

Writing the series expansion of these two symbols using $(1-z)^{-1/2}$ for $z = k^2/|\xi|^2$ and $(1-z)^{1/2}$ for $z = {k_\varepsilon}^2/|\xi|^2$ in the elliptic part of the operators (for $|\xi| \to +\infty$), we obtain

$$\sigma_p(L) = -\frac{1}{2|\xi|}(1+\sum_{\ell=1}^{+\infty}\frac{L_\ell}{|\xi|^{2\ell}}) \text{ and } \sigma_p(\mathbf{\Lambda}_\varepsilon) = \frac{k}{k_\varepsilon}|\xi|(1+\sum_{\ell=1}^{+\infty}\frac{\lambda_\ell}{|\xi|^{2\ell}}),$$

for some complex numbers L_ℓ and λ_ℓ depending on $\ell \in \mathbb{N}^*$, k and ε. This implies that the principal symbol of the composition of these two operators can be written as

$$\sigma_p(-L\mathbf{\Lambda}_\varepsilon) = \frac{k}{2k_\varepsilon} + \sum_{\ell=1}^{+\infty}\frac{d_\ell}{|\xi|^{2\ell}},$$

for some complex coefficients d_ℓ, with $\ell \in \mathbb{N}^*$. Finally, the operator $-L\mathbf{\Lambda}_\varepsilon$ takes the form

$$-L\mathbf{\Lambda}_\varepsilon = \frac{k}{2k_\varepsilon}I + \widetilde{K}, \tag{5.3}$$

with $\widetilde{K}$ a compact operator of negative order. (This latter relation can be compared in a certain sense to the Caldèron's relation $-2LD = I/2 - 2M^2$ [24, 25]). Returning to the operator $B_{D,\varepsilon}$, we deduce from the above result that

$$B_{D,\varepsilon} = aI + K,$$

where the complex number $a = 1/2 + k/(2k_\varepsilon) \neq 0$ for $k > 0$ and $K = -M + \widetilde{K}$ is a compact perturbation since it is the sum of two compact operators from $H^{1/2}(\Gamma)$.

Since the operator $B_{D,\varepsilon}$ arising in (5.2) is a second-kind Fredholm operator, the Riesz-Fredholm theory classically yields its inversibility if the operator is injective. Therefore, it is sufficient to prove that the homogeneous equation associated to (5.2) admits $\psi = 0$ as unique solution to get the existence and uniqueness of the solution to the generalized Brakhage-Werner integral equation (5.2). Let $\psi \in H^{1/2}(\Gamma)$ solution to $B_{D,\varepsilon}\psi = 0$. Then, the function u^+ defined by

$$u^+(x) = -M\psi(x) - L\mathbf{\Lambda}_\varepsilon\psi(x), \quad \forall x \in \Omega^+,$$

is solution to the homogeneous exterior Dirichlet problem and $u^+ = 0$ in Ω^+. Using Proposition 2.1, one gets

$$-\gamma_0^- u^- = \psi, \text{ in } H^{1/2}(\Gamma) \quad \text{and} \quad -\gamma_1^- u^- = \mathbf{\Lambda}_\varepsilon\psi, \text{ in } H^{-1/2}(\Gamma).$$

The first Green formula in the interior domain Ω^- gives

$$< \gamma_0^- u^-, \gamma_1^- u^- >_\Gamma = \int_{\Omega^-} |\nabla u^-|^2 - k^2|u^-|^2 d\Omega^-,$$

where $< f, g >_\Gamma$ designates the duality product of two functions $f \in H^{1/2}(\Gamma)$ and $g \in H^{-1/2}(\Gamma)$. If we take the imaginary part of this equation, we obtain the relation $\Im(< \psi, \Lambda_\varepsilon \psi >_\Gamma) = 0$. From the definition of the square-root operator $\mathbf{\Lambda}_\varepsilon$, we have the spectral decomposition

$$\mathbf{\Lambda}_\varepsilon \psi = ik \sum_{j=1}^{+\infty} \sqrt{1 - \frac{\mu_j}{k_\varepsilon^2}} \psi_j \phi_j, \quad \text{with } \psi = \sum_{j=1}^{+\infty} \psi_j \phi_j.$$

Since $\{\phi_j\}_{j \in \mathbb{N}^*}$ is an orthonormal basis, we obtain that the imaginary part is given by

$$\Im(< \psi, \mathbf{\Lambda}_\varepsilon \psi >_\Gamma) = k \sum_{j=1}^{+\infty} \Re(\sqrt{1 - \frac{\mu_j}{k_\varepsilon^2}}) |\psi_j|^2 = 0. \tag{5.4}$$

Using that $\mu_j > 0$ for $j \in \mathbb{N}^*$, we can easily prove that $\Re(\sqrt{1 - \mu_j / k_\varepsilon^2}) > 0$ for $k > 0$ and $\varepsilon > 0$. Finally, relation (5.4) gives that $\psi_j = 0$ for all $j \in \mathbb{N}^*$ and hence $\psi = 0$. This ends the proof of proposition 5.2. □

5.3. The sound-hard scattering problem. The generalized BW integral equation to solve for the Neumann problem is written as

$$B_{N,\varepsilon} \varphi = g, \text{ in } H^{-1/2}(\Gamma), \tag{5.5}$$

where $B_{N,\varepsilon} = I/2 - N - D\mathbf{V}_\varepsilon$. Then, we have the existence and uniqueness of the solution to this latter equation.

PROPOSITION 5.3. *The generalized BW integral equation (5.5) admits one and only one solution for any wavenumber $k > 0$ and damping parameter $\varepsilon > 0$.*

Proof. We do not detail the proof which follows similar arguments as for the Dirichlet problem. □

One of the most important properties of the integral equation (5.5) is that it is defined by a second-kind integral operator. This is not the case of the usual Brakhage-Werner integral equation for the Neumann problem. This aspect can be understood easily if $\mathbf{V}_\varepsilon$ is replaced by $-i/k$ in (5.5). Indeed, since the operator D is a first-order pseudodifferential operator, $D\mathbf{V}_\varepsilon$ is a second-kind integral operator because $\mathbf{V}_\varepsilon$ is a pseudodifferential operator of order -1 whose principal symbol is almost the inverse of $\sigma_p(D)$. This is not the case of the approximation $-iD/k$ which remains a first-order pseudodifferential operator. As seen below, this property is essential from a numerical point of view since second-kind integral equations of the form $aI + K$ are characterized by an eigenvalue clustering around a for $|\xi| \to +\infty$ if K is compact and $a \neq 0$. This last property is essential for a good behaviour of a Krylov iterative solver as e.g. the GMRES [13, 35, 41]. Let us notice that the situation is different for a Dirichlet boundary condition. The operator B_D is already a compact perturbation of the identity operator even for the usual formulation. A better eigenvalues clustering is expected for $B_{D,\varepsilon}$ by choosing the operator $\mathbf{\Lambda}_\varepsilon$. We will see during the numerical experiments that the most visible improvements are given for the Neumann problem.

6. The example of the sphere. Let $\Gamma = S_1$ be the sphere of radius 1 centered at the origin. A classical result [26] shows that $\mu_\ell = -\ell(\ell+1)$ are the eigenvalues of Δ_{S_1}. The subspace spanned by the eigenfunctions of Δ_{S_1} has a dimension equal to $2\ell + 1$. Let us introduce the spherical harmonics $Y_{\ell m}$ as the functions defined by

$$Y_{\ell m}(\hat{\theta}) = \left[\frac{2\ell+1}{4\pi} \frac{(\ell - |m|)!}{(\ell + |m|)!} \right]^{1/2} P_\ell^m(\cos\theta) e^{im\phi},$$

for $\ell = 0, 1, 2, ..., -\ell \leq m \leq \ell$, and P_ℓ^m the associated Legendre polynomials. Here, we have defined $(r, \hat{\theta})$ as the spherical polar coordinate system such that $\hat{\theta} = (\theta, \phi) \in S_1$. The functions $Y_{\ell m}$, for $\ell = 0, 1, 2, ..., -\ell \leq m \leq \ell$, constitue an orthonormal basis for $L^2(S_1)$. In addition, they also form a basis of eigenvectors for the four integral operators L, M, N and D. If j_ℓ and $h_\ell^{(1)}$ are respectively the spherical Bessel and first-kind Hankel functions of order ℓ, we have the following proposition (see [1, 36]).

PROPOSITION 6.1. *The eigenvalues $\mathcal{L}_\ell$, $\mathcal{M}_\ell$, $\mathcal{N}_\ell$ and $\mathcal{D}_\ell$ of multiplicity $(2\ell + 1)$ respectively associated with the elementary integral operators L, M, N and D are given by*

$$\begin{aligned} &LY_{\ell m} = \mathcal{L}_\ell Y_{\ell m} = \{ikj_\ell(k)h_\ell^{(1)}(k)\}Y_{\ell m}, \\ &MY_{\ell m} = \{\frac{1}{2} - ik^2 j_\ell'(k)h_\ell^{(1)}(k)\}Y_{\ell m}, \qquad \mathcal{N}_\ell Y_{\ell m} = -\mathcal{M}_\ell Y_{\ell m}, \\ &DY_{\ell m} = \mathcal{D}_\ell Y_{\ell m} = \{-ik^3 j_\ell'(k)(h_\ell^{(1)})'(k)\}Y_{\ell m}, \end{aligned} \tag{6.1}$$

for $\ell = 0, 1, 2, ..., -\ell \leq m \leq \ell$.

A direct computation gives the eigenvalues $\mathcal{B}_{D,\varepsilon}^\ell$ and $\mathcal{B}_{N,\varepsilon}^\ell$ of respectively the operators $B_{D,\varepsilon}$ and $B_{N,\varepsilon}$

$$B_{D,\varepsilon} Y_{\ell m} = \mathcal{B}_{D,\varepsilon}^\ell Y_{\ell m} = \left((\frac{1}{2} - M_\ell) - L_\ell \mathbf{\Lambda}_{\varepsilon\ell}\right) Y_{\ell m}$$

and

$$B_{N,\varepsilon} Y_{\ell m} = \mathcal{B}_{N,\varepsilon}^\ell Y_{\ell m} = \left((\frac{1}{2} - N_\ell) - D_\ell \mathbf{V}_{\varepsilon\ell}\right) Y_{\ell m},$$

setting $\mathbf{\Lambda}_{\varepsilon\ell} = ik\sqrt{1 - \mu_\ell / k_\varepsilon^2}$ and $\mathbf{V}_{\varepsilon\ell} = \mathbf{\Lambda}_{\varepsilon\ell}^{-1}$, for $\ell = 0, 1, 2, ..., -\ell \leq m \leq \ell$.

To illustrate the repartition of the eigenvalues of the integral operators, we draw on Fig. 6.1 the spectrum of both the usual and generalized Brakhage-Werner operators for the unit sphere. For the usual Brakhage-Werner integral operator (left figure), we observe a small cluster of eigenvalues linked to the low-order modes (hyperbolic part of the operator [7]). A large number of eigenvalues corresponding to the evanescent modes (high-order spatial modes) are on the line $x = 1/2$. This repartition of eigenvalues penalizes the convergence rate of the GMRES. This problems is avoided with the new operator. Eigenvalues clustering occurs for both the low and high-order harmonics. Just a few eigenvalues corresponding to the coupling between low and high-order modes is observable as a loop around 1. This eigenvalues clustering is a characteristic of a second-kind Fredholm operator.

7. Generalized Combined Field Integral Equations. This section is devoted to a generalization of the Combined Field Integral Equation introduced by Harrington and Mautz in electromagnetism [30, 22]. This generalization is particularized to the case of the scattering problem of an electromagnetic wave by a perfectly conducting body for a TM or a TE polarized wave. Therefore, we are led to solve the two-dimensional Helmholtz equation with respectively a Dirichlet or a Neumann boundary condition. The extension to the three-dimensional acoustic problem is simply a transcription of the two-dimensional equations. The case of the full Maxwell equations will be studied somewhere else and is beyond the scope of the present paper.

Let us begin by recalling some basic results (see e.g. [22]). Let $\mathbf{j}$ be the electric surfacic current representing the jump of the tangential component of the magnetic

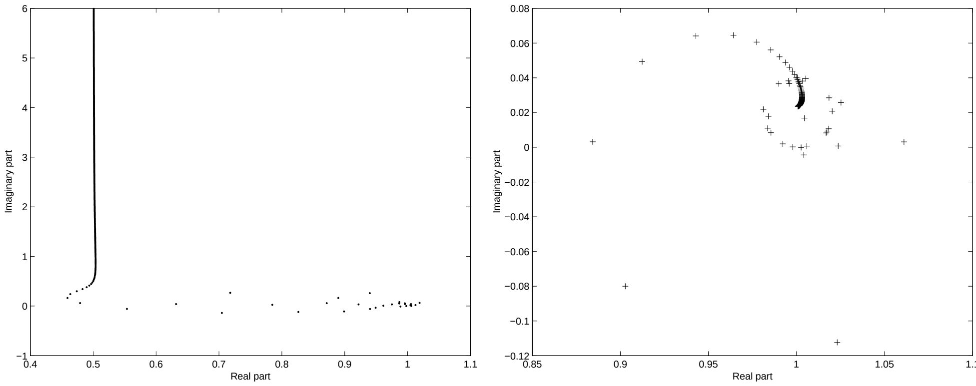

FIG. 6.1. *Sound-hard sphere: Eigenvalues of the usual (left) and generalized (right) Brakhage-Werner integral operators for a frequency $k = 25$ and $m = 24$.*

field through the interface Γ of Ω^-. By determinating $\mathbf{j}$, we can compute both the electric and magnetic scattered fields from the integral representation theorems for the Maxwell equations. The current $\mathbf{j}$ is solution to the Electric and Magnetic Field Integral Equations (EFIE and MFIE). However, for a closed surface, these integral equations admit some resonance frequencies and are ill-posed. To overcome this problem, Harrington and Mautz propose to consider a Combined Field Integral Equation (CFIE) resulting from a convex combination between the EFIE and MFIE. More precisely, the usual CFIE is given by

$$\text{CFIE} = \alpha\text{EFIE} + (1-\alpha)\frac{i}{k}\text{MFIE}. \tag{7.1}$$

The coupling parameter α is numerically estimated for minimizing the condition number of the CFIE. We precise different values during the numerical experiments. In the case of a TM polarized wave (Dirichlet), the EFIE and the MFIE are respectively given by

$$Lp = -\gamma_0^+ u^{\text{inc}} \quad \text{and} \quad \left(\frac{I}{2} + N\right) p = -\gamma_1^+ u^{\text{inc}}. \tag{7.2}$$

For a TE polarized wave (Neumann), we have the two integral equations

$$D\phi = -\gamma_1^+ u^{\text{inc}} \quad \text{and} \quad \left(\frac{I}{2} + M\right) \phi = -\gamma_0^+ u^{\text{inc}}. \tag{7.3}$$

In the above equations, we have set $p = \gamma_1^+ u^+ - \gamma_1^- u^-$ and $\phi = \gamma_0^+ u^+ - \gamma_0^- u^-$. For acoustic field radiation problems, ϕ and p respectively represent the jump of the pressure and the normal component of the velocity through the boundary Γ. Unlike the Brakhage-Werner integral formulations, the CFIE hence involves some physical unknown densities.

We propose here to generalize the usual CFIE by firstly regularizing the EFIE by the pseudodifferential operator $\mathbf{\Lambda}_\varepsilon$ or $\mathbf{V}_\varepsilon$ according to the polarization and next adding the MFIE. As a by product, the composition operator resulting from the first step yields a compact perturbation of the identity operator. More precisely, let us consider the Dirichlet boundary value problem. Then, the generalized CFIE that we consider is stated as

$$C_{D,\varepsilon} p = h_{D,\varepsilon}, \quad \text{in } H^{-1/2}(\Gamma), \tag{7.4}$$

where we have set $C_{D,\varepsilon}$ as the integrodifferential operator defined by

$$C_{D,\varepsilon} = (I + \frac{N}{2}) - \mathbf{\Lambda}_\varepsilon L$$

and where the right-hand side is given by: $h_{D,\varepsilon} = -(\gamma_1^+ - \mathbf{\Lambda}_\varepsilon \gamma_0^+)u^{\text{inc}}$. We straightforwardly prove that the operator $C_{D,\varepsilon}$ is the Hermitian adjoint of $B_{D,\varepsilon}$ given by (5.2). Hence, the equation (7.4) is uniquely solvable at any positive frequency under the same condition as Proposition 5.2. In the usual CFIE (7.1), a coupling parameter α is incorporated in the convex combination. Here, a numerical study shows that $\alpha = 0.5$ is the best (natural) choice for the new formulations. For this reason, we do not take this parameter into account.

Concerning the Neumann problem, we consider the following generalization of the CFIE

$$C_{N,\varepsilon} \phi = h_{N,\varepsilon}, \quad \text{in } H^{1/2}(\Gamma), \tag{7.5}$$

defining $C_{D,\varepsilon}$ as the operator

$$C_{N,\varepsilon} = (I + \frac{M}{2}) - \mathbf{V}_\varepsilon D \tag{7.6}$$

and setting: $h_{N,\varepsilon} = -(\gamma_0^+ - \mathbf{V}_\varepsilon \gamma_1^+)u^{\text{inc}}$. The well-posedness of the equation (7.5) at any frequency $k > 0$ is a consequence of Proposition 5.3 by still noticing that the operator $C_{N,\varepsilon}$ given by (7.6) is the Hermitian adjoint operator of the integral operator $B_{N,\varepsilon}$ defined by relation (5.5). As the usual CFIE, the unknown field p or ϕ is a physical quantity unlike the case of the generalized Brakhage-Werner integral equations.

8. Approximation and numerical implementation in a Krylov iterative solver. We only detail here the adopted strategy for the resolution of the generalized Brakhage-Werner integral equation for the Dirichlet problem which is given by

$$B_{D,\varepsilon} \psi = g, \quad \text{in } H^{1/2}(\Gamma) \tag{8.1}$$

where the integral operator $B_{D,\varepsilon}$ is

$$B_{D,\varepsilon} = (\frac{I}{2} - M) - L \mathbf{\Lambda}_\varepsilon \tag{8.2}$$

and where $g = -u^{\text{inc}}$ on Γ. The other kinds of generalized equations can be treated using a similar adapted approach. Moreover, we just give the developments required for the three-dimensional case, the extension to the two-dimensional case being direct.

Let us introduce a triangularization $\mathcal{T}_h = \cup_{j=1}^{N_T} T$ of Γ based on triangles. The polyedric interpolated surface is denoted by Γ_h. We define the total number of triangles by N_T and the total number of vertices by N_V. Our approximation is based on a linear Galerkin boundary element method even if other approaches can be *a priori* developed. To this end, let us introduce the following approximation space

$$V_h = \{\phi_h \in \mathcal{C}^0(\Gamma_h); \phi_T = \phi_{h|T} \in \mathbb{P}_1, \forall T \in \mathcal{T}_h\}.$$

As a consequence, we have $\dim V_h = N_V$. If $h_{\max}$ is the maximal length of the edges of the triangles involved in $\mathcal{T}_h$, then $n_\lambda = \lambda/h_{\max}$ designates the density of discretization points per wavelength. In the sequel, if Z is an integral or a differential operator, we denote by $[Z]$ the discretized matrix associated to the linear discretization of Z. Following this approximation, the discretization of (8.1)-(8.2) leads to the resolution of the dense complex non-hermitian linear system of equations

$$[B_{D,\varepsilon}]\boldsymbol{\psi}_h = \mathbf{g}_h, \text{ with } [B_{D,\varepsilon}] = (\frac{[I]}{2} - [M]) - [L][\boldsymbol{\Lambda}_\varepsilon]. \tag{8.3}$$

The complex valued vectors $\boldsymbol{\psi}_h$ and $\mathbf{g}_h$ are elements of $\mathbb{C}^{N_V}$. They are respectively the $\mathbb{P}_1$-interpolation of the unknown density ψ and of the right hand side g. Concerning the evaluation of the integral operators M and L, we have used their weak variational formulations while the approximation $[I]$ of the identity operator I is just the mass matrix. A suitable approximation and fast evaluation of the pseudodifferential operator $\boldsymbol{\Lambda}_\varepsilon$ is detailled below.

Since we are dealing with the resolution of a second-kind Fredholm integral equation [13, 35, 41], we consider the GMRES procedure without restart [43, 44] as Krylov iterative solver for the solution of (8.3). The GMRES requires one matrix-vector product at each iteration. It is now well-known that a direct evaluation of a matrix-vector product needs $\mathcal{O}(N_V^2)$ operations (option taken in the paper) and that the Fast Multipole Method (FMM) leads to an efficient evaluation in $\mathcal{O}(N_V \log N_V)$ operations. However, we are rather interested here in the convergence rate of the GMRES for the different kinds of integral equations. This implies that a good qualitative parameter to measure it is given by the total number of matrix-vector products to get an *a priori* fixed tolerance *tol* in the GMRES. However, this remark is valid if the application of the pseudodifferential operator $\boldsymbol{\Lambda}_\varepsilon$ is efficiently realized. Let us now detail both its approximation and implementation.

The discretization of the pseudodifferential operator $\boldsymbol{\Lambda}_\varepsilon$ is not straightforward. Moreover, the matrix which corresponds to the numerical discretization of the non-local operator leads to a dense complex matrix. Hence, the application of this matrix to a vector $\mathbf{x} \in \mathbb{C}^{N_V}$ needs a $\mathcal{O}(N_V^2)$ computational cost. To realize a suitable and efficient implementation, we proceed as in the BPM methods using a paraxial approximation of the square-root operator. To this end, we must be able to simulate the pseudodifferential operator $\boldsymbol{\Lambda}_\varepsilon = ik\sqrt{1+X}$ for the partial differential operator $X = \Delta_\Gamma/k_\varepsilon^2$, for a small value of ε and any spatial frequency. We propose to follow the rotating branch-cut technique introduced by Milinazzo *et al.* [40] for the modeling of underwater acoustic wave propagation and latter used in the OSRC context for acoustic scattering [8]. More precisely, this approximation is defined by

$$\sqrt{1+X} \approx e^{i\theta/2} R_p(e^{-i\theta}X) = A_0 + \sum_{j=1}^{p} \frac{A_j X}{1+B_j X},$$

where the complex valued constants A_0, A_j and B_j are given by

$$A_0 = e^{i\theta/2} R_p(e^{-i\theta}X), \quad A_j = \frac{e^{-i\theta/2} a_j}{(1+b_j(e^{-i\theta}-1))^2} \quad \text{and} \quad B_j = \frac{e^{-i\theta} b_j}{(1+b_j(e^{-i\theta}-1))}.$$

Hereabove, R_p denotes the usual Padé approximant of order p with branch-cut along

$\{z \in \mathbb{C}; z < -1\}$

$$R_p(z) = 1 + \sum_{j=1}^{p} \frac{a_j z}{1 + b_j z}$$

setting

$$a_j = \frac{2}{2p+1} \sin^2(\frac{j\pi}{2p+1}) \text{ and } b_j = \cos^2(\frac{j\pi}{2p+1}).$$

The angle θ allows to rotate the branch-cut $\{z \in \mathbb{C}; z < -1\}$ and to position it along the ray $z = -1 + re^{i(\theta+\pi)}$. In [8], we show that the parameters $p = 8$ and $\theta = \pi/3$ yield a satisfactory approximation of the exact square-root operator. Following [8], we are led to solve p Helmholtz-type partial differential equations on Γ which are approximated by linear surface finite elements in a variational way [4]. Therefore, at each step of the GMRES, we compute in an approximate way the image $\mathbf{y}$ of a vector $\mathbf{x} \in \mathbb{C}^{N_V}$ by $[\mathbf{\Lambda}_\varepsilon]$ firstly solving p highly sparse decoupled linear systems (eventually parallelized on different processors)

$$(\frac{B_j}{k_\varepsilon^2}[\Delta_\Gamma] + [I])\mathbf{x}_j = \mathbf{x}, \quad j = 1, ..., p, \tag{8.4}$$

and next computing

$$\mathbf{y} = ik(A_0[I]\mathbf{x} + \sum_{j=1}^{p} A_j[\Delta_\Gamma]\mathbf{x}_j). \tag{8.5}$$

The matrix $[\Delta_\Gamma]$ represents the rigidity matrix on Γ_h. The resolution of the p linear systems given by (8.4) is done by GMRES without restart and preconditioned by ILUT with a threshold parameter equal to 10^{-2} for a tolerance 10^{-8}. The convergence for the resolution of each system requires 2 or 3 iterations. Finally, the resulting cost of this procedure is linear and asymptotically equivalent to $\mathcal{O}(pN_V)$. This cost is negligeable compared to the usual cost $\mathcal{O}(N_V \log N_V)$ of a matrix-vector product in the FMM since p is relatively small.

9. Numerical results. We present some numerical results to compare the different kinds of integral formulations. We consider an incident plane wave

$$u^{\text{inc}}(x) := \exp(ik\boldsymbol{\nu} \cdot x),$$

where $\boldsymbol{\nu}$ denotes the vector of incidence in circular or spherical coordinates.

9.1. Two-dimensional case. In the case of a Dirichlet datum, we compare the four following integral representations: the usual and generalized Brakhage-Werner (BW) formulations (respectively given by the equation (3.2) for $\eta = ik$ and (5.2)), the usual and generalized Combined Field Integral Equations (CFIE) given by formulations (7.1)-(7.2) and (7.4). The α parameter defining the usual CFIE is taken as $\alpha = 0.3$. Since for a Dirichlet boundary condition, all the integral equations are some second-kind Fredholm equations, the condition number does not depend on the discretization step (through for instance the density of discretization points per wavelength) and an eigenvalue clustering occurs for the high-order spatial modes. However, a slight frequency dependence of the condition number should be observable [7, 22].

As previously noticed, we consider that the number of matrix-vector products is a good measure to estimate the convergence rate of the GMRES. The GMRES Krylov iterative solver without restart and with a tolerance $tol = 10^{-8}$ is used during the numerical simulations. We present on Fig. 9.1 two examples of computations for the scattering of an incident plane wave of incidence zero degree on an elliptical cylinder of semi-axis a and b along respectively the x_1 and x_2-directions. We have fixed $a = 1$ and b is taken equal to 0.01 on the left and $b = 0.05$ on the right figures. The density of discretization points is $n_\lambda = 24$. In both cases, we see that the generalized versions provide a better convergence rate compared to the usual formulations. The difference is more observable for the first test case. This is due to the stronger curvature effects which are taken into account in the new formulations through the Laplace-Beltrami operator Δ_Γ. Among the four formulations, the generalized Brakhage-Werner formulation seems to be the most efficient. Other tests for different geometries confirm this conclusion.

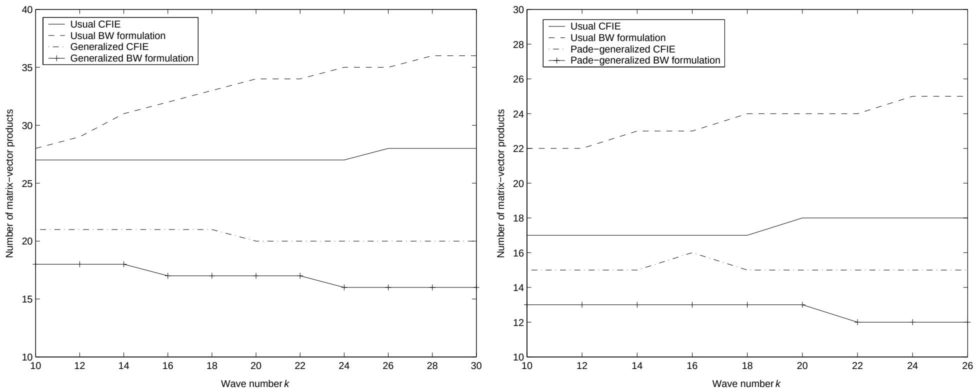

FIG. 9.1. *Sound-soft elliptical cylinder: number of matrix-vector products for the four integral formulations with respect to the wave number k.*

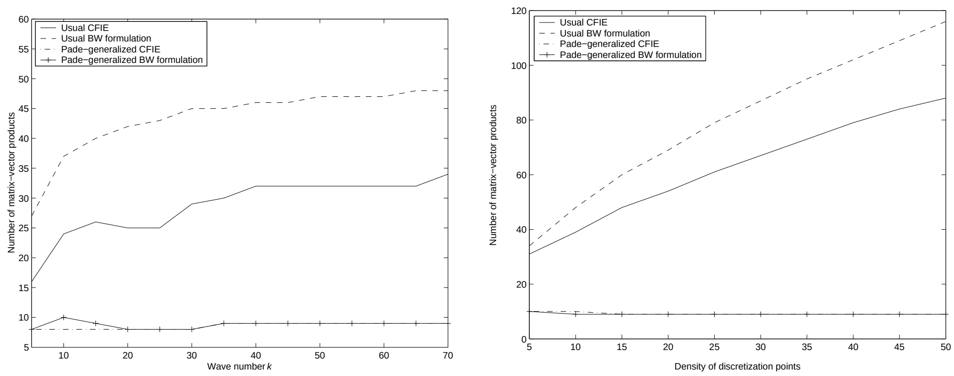

FIG. 9.2. *Sound-hard elliptical cylinder: number of matrix-vector products for the four integral formulations with respect to the wave number k (left: $n_\lambda = 10$ and zero degree incidence) and the density n_λ of discretization points per wavelength (right: $k = 15$ and zero degree incidence).*

Let us consider a Neumann boundary condition. The four integral formulations under consideration are now: the usual and generalized Brakhage-Werner formulations given respectively by (3.7) (for $\widetilde{\mathbf{V}} = -i/k$) and (5.5), the usual and Generalized CFIE (7.3) and (7.5) (taking now $\alpha = 0.2$). As for the sound-soft case, we can expect that the condition number is a function of the wavenumber. Unlike the generalized formulations, the usual BW and CFIE integral equations are not some second-kind Fredholm integral equations. Therefore, the condition number is linearly dependent with respect to the density n_λ of discretization points per wavelength. Moreover, no eigenvalue clustering occurs in the zone of high-order spatial frequencies (see for instance [7, 28] and Figure 6.1 for the sphere). To illustrate the impact of these properties on the convergence rate of the iterative solver, we consider on Fig. 9.2 the scattering problem of a plane wave of incidence zero degree on the elliptical cylinder of characteristics $a = 1$ and $b = 0.25$. We observe respectively on the left and right figures that the generalized formulations lead to an important reduction of the number of matrix-vector products compared to the usual formulations when the wavenumber k or the density n_λ increases. This cost is even independent of these two parameters. These conclusions are still true on Fig. 9.3 where we consider an incident plane wave of incidence 45 degrees on the square cylinder centered at the origin and with a sidelength equal to 2.

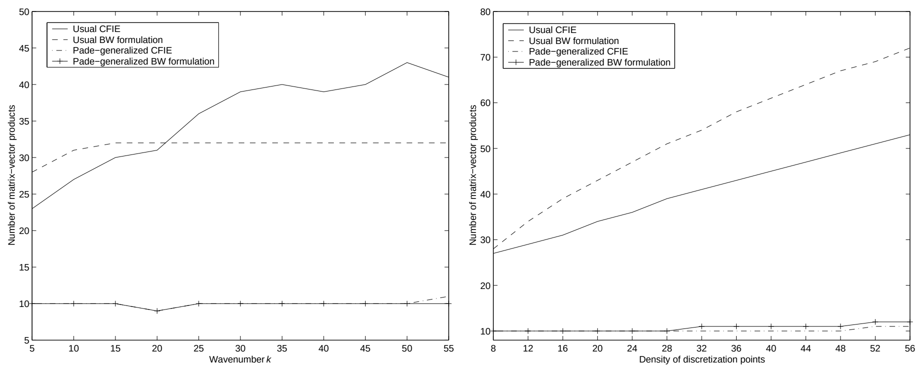

FIG. 9.3. *Sound-hard square cylinder: number of matrix-vector products for the four integral formulations with respect to the wave number k (left: $n_\lambda = 10$ and 45 degrees incidence) and the density n_λ of discretization points per wavelength (right: $k = 10$ and 45 degrees incidence).*

To end this section on the two-dimensional computations, we present on Figure 9.4 the scattering problem by a non-convex obstacle: a square cylinder with a reentrant square cavity. The domain is defined as the previous square cylinder but without the square whose vertices are given by the four coordinates: $(-1, 0.4)$, $(0, 0.4)$, $(0, -0.4)$ and $(-1, -0.4)$. The incident plane wave has an incidence angle equal to 30 degrees and strikes into the cavity. Therefore, the field is multiply scattered into the cavity. As it can be seen on the left picture of figure 9.4, it seems that it does not affect the fact that the number of iterations is independent on n_λ. However, we can observe that the total number of iterations increases weakly according to k even if the new formulations have a better convergence rate. This small deterioration can be seen as one aspect to improve concerning the way of constructing an alternative formulation (this aspect also arises for the Dirichlet data). However, if one compares the generalized integral formulations to the usual one, we can clearly conclude to the better convergence properties of the new formulations.

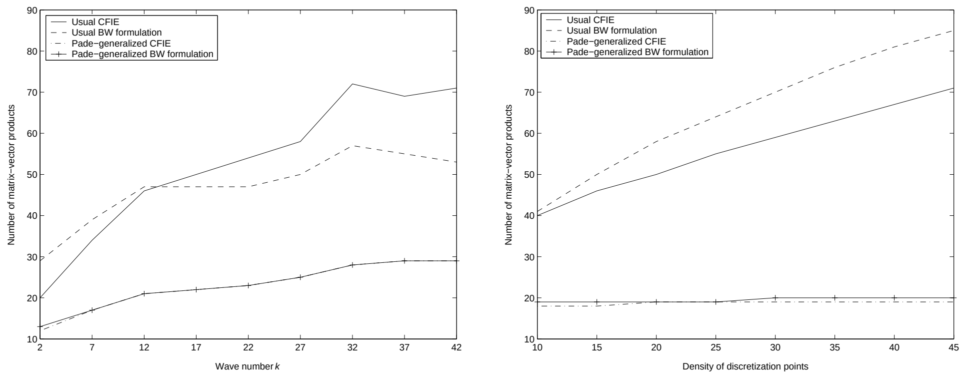

FIG. 9.4. *Sound-hard square cylinder with cavity: number of matrix-vector products for the four integral formulations with respect to the wave number k (left: $n_\lambda = 10$ and 30 degrees incidence) and the density n_λ of discretization points per wavelength (right: $k = 10$ and 30 degrees incidence).*

9.2. Three-dimensional case. The tolerance of the GMRES is now fixed to $tol = 10^{-6}$. We consider an incident plane wave of incidence zero degree illuminating the sound-soft unit sphere centered at the origin. We take $\alpha = 0.2$ in the classical CFIE. We report on Fig. 9.5 the evolution of the number of matrix-vector products according to k for a density of discretization points per wavelength $n_\lambda = 10$. We observe that the generalized formulations exhibit a better behaviour according to k than the usual ones.

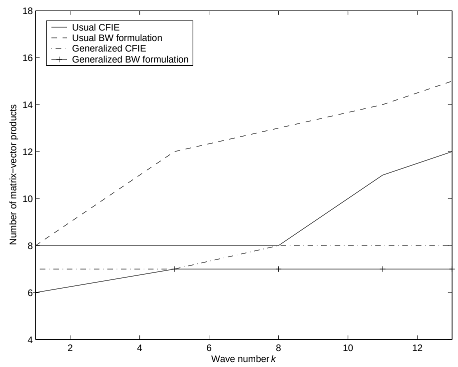

FIG. 9.5. *Sound-soft unit sphere: number of matrix-vector products for the four integral formulations with respect to the wave number k.*

Let us now compare the generalized formulations versus the usual integral equations for the sound-hard scattering problem. On Fig. 9.6 and 9.7, we respectively report the scattering problem of a plane wave of incidence zero degree by the unit sphere and an ellipsoidal scatterer of semi-axis $a = 1$ and $b = c = 0.5$ respectively along the x_1-, x_2- and x_3-directions and centered at the origin. Once again, we see that the new formulations lead to a better convergence rate of the iterative solver. Unlike the generalized formulations, the number of iterations of the usual formulations depends on the density n_λ. Moreover, we observe a better behaviour of the generalized formulations than the classical ones according to the wave number. These results extend the ones obtained in the two-dimensional case.

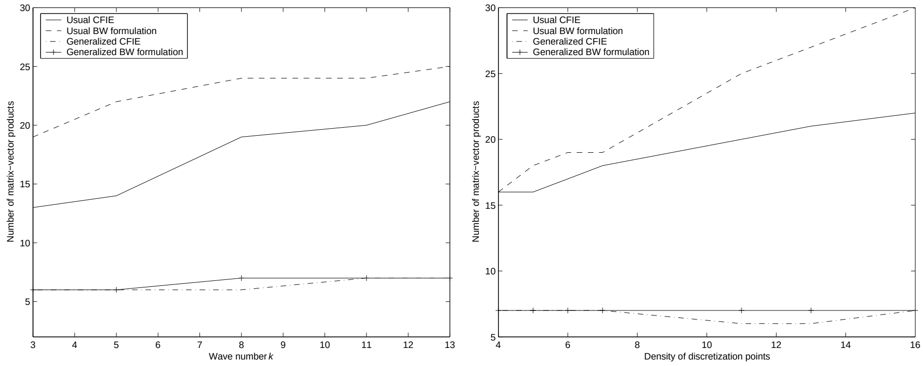

FIG. 9.6. *Sound-hard unit sphere: number of matrix-vector products for the four integral formulations with respect to the wave number k (left:* $n_\lambda = 10$ *and zero degree incidence) and the density of discretization points per wavelength (right:* $k = 10$ *and zero degree incidence).*

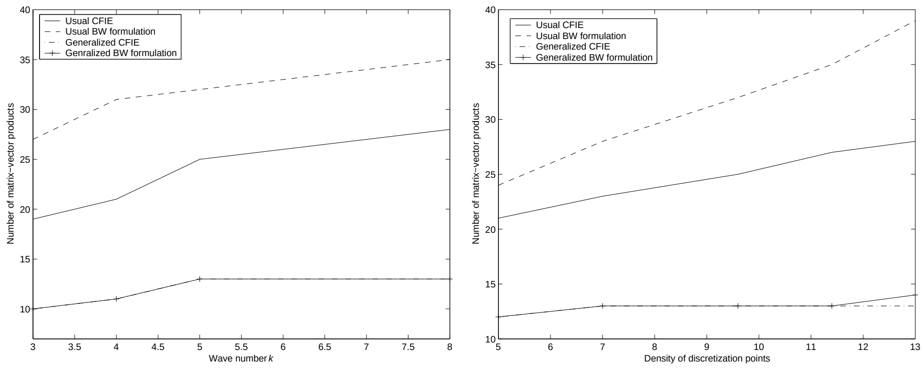

FIG. 9.7. *Sound-hard ellipsoidal scatterer: number of matrix-vector products for the four integral formulations with respect to the wave number k (left:* $n_\lambda = 10$ *and zero degree incidence) and the density of discretization points per wavelength (right:* $k = 5$ *and zero degree incidence).*

Finally, we take as scatterer the cube centered at the origin and with a sidelength equal to 2. The spherical angle of incidence is $(0, 30)$ degrees. For this test-case, we have observed a lack of accuracy for the usual CFIE if the α parameter is not well-chosen. To clarify the results, we consider two possible choices: for $\alpha = 0.2$ we obtain a better condition number (and less iterations) but a lack of accuracy of the computed solution and for $\alpha = 0.5$ we get a good accuracy but to the detriment of the convergence rate. For $\alpha = 0.5$, the resulting equation is nothing else than the transposed BW formulation and therefore have the same convergence rate. All the remarks of the two previous three-dimensional cases extend to the cube.

10. Conclusion. We have proposed in this paper some alternative well-posed integral equations for the scattering problem by a closed surface. These formulations which generalize the usual Brakhage-Werner and CFIE integral equations have an improved convergence rate when they are solved by a Krylov subspace iterative solver. Their convergence rate is independent of the density of discretization points per wavelength and almost of the frequency. These new formulations should be efficient when

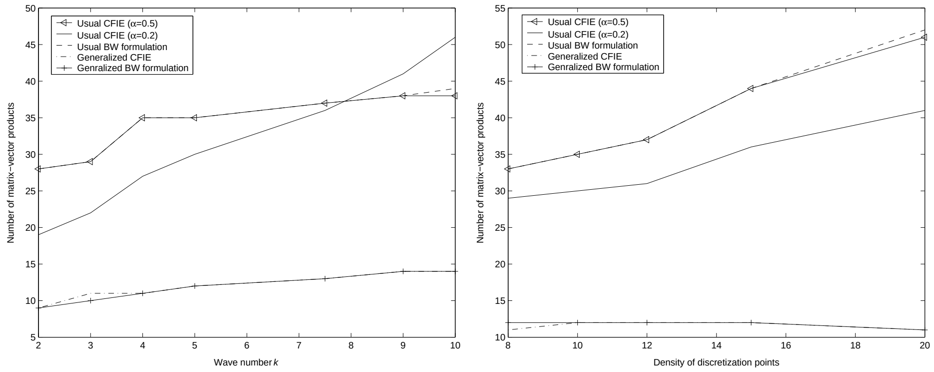

FIG. 9.8. *Sound-hard unit cube: number of matrix-vector products for the four integral formulations with respect to the wave number k (left: $n_\lambda = 10$ and incidence $(0, 30)$) and the density of discretization points per wavelength (right: $k = 5$ and incidence $(0, 30)$).*

they are coupled to a fast solver like for instance the FMM [22, 42] or the high-order solvers developed in [10, 11].

The extension to more general scattering problems is actually under progress (generalized impedance boundary conditions for instance). Moreover, more numerical experiments remain to do for higher frequencies and more complicate shapes to confirm the efficiency of the alternative formulations. The extension to the three-dimensional system of Maxwell' equations is currently being explored.

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