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problems based on the pole condition:
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Summary In this paper we study the PML method for Helmholtz-type scattering problems with radially symmetric potential. The PML method consists in surrounding the computational domain by a **P**erfectly **M**atched sponge **L**ayer. We prove that the approximate solution obtained by the PML method converges exponentially fast to the true solution in the computational domain as the thickness of the sponge layer tends to infinity. This is a generalization of results by Lassas and Somersalo based on boundary integral equation techniques. Here we use techniques based on the pole condition instead. This makes it possible to treat problems without an explicitly known fundamental solution.

Key words transparent boundary conditions, PML, pole condition

Mathematics Subject Classification (1991): 65N12

1 Introduction

Since the first paper by Bérenger in 1994 ([1]), the Perfectly Matched Layer (PML) method has become very popular due to its accuracy, simplicity and flexibility. In this paper we explore the connections between the PML method for time-harmonic scattering problems and the methods based on the pole condition, which are discussed in [4].

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We start with a brief summary of the derivation of the PML equations. Let $u(r, \hat{x})$ denote the solution to the scattering problem in a coordinate system consisting of a radial variable $r > 0$ and a vector of angular variables \hat{x} . The first step of the PML method consists in a complex extension of the solution $u(\cdot, \hat{x})$ along some given path $\gamma : [a, \infty) \rightarrow \mathbb{C}$, $a > 0$ which satisfies

$$\gamma(a) = a, \Re \gamma(r) = r, \text{ and } \Im \gamma' \geq 0.$$

In cartesian coordinates the so-called Bérenger solution $u^{(B)}(r, \hat{x}) := u(\gamma(r), \hat{x})$ satisfies a Helmholtz-type equation with an anisotropic damping tensor. If u is outgoing, then $u^{(B)}(r, \hat{x})$ decays exponentially as $r \rightarrow \infty$. On the other hand, $u^{(B)}(r, \hat{x})$ grows exponentially if u is an incoming field. Therefore, the Sommerfeld radiation condition for u is equivalent to the boundedness of $u^{(B)}(r, \hat{x})$. In a second step, the boundedness condition for $u^{(B)}(r, \hat{x})$ is replaced by the zero Dirichlet condition $u^{(B)}(\rho, \hat{x}) = 0$ at some finite distance $\rho > a$. We end up with an elliptic boundary value problem on a bounded domain, which can be solved by standard finite element codes.

The analysis of this paper is based on the work of Collino and Monk [2] and Lassas and Somersalo [8]. We show that for the Helmholtz equation with a radially symmetric potential the solution to the PML equations converge exponentially to the true solution within the ball $\{x : |x| < a\}$ as $\rho \rightarrow \infty$. In [7] Lassas and Somersalo show the exponential convergence of the PML method for general convex computational domains, but constant exterior potentials. Our proof proceeds along the same lines as in [8], but we replace integral equation techniques by the representation formula derived in [4]. This allows us to treat problems for which no fundamental solution is known explicitly. In particular, as shown in numerical experiments the method converges for general convex domains and more general inhomogeneous exterior domains as waveguide structures, see [11, 5, 6]. Unfortunately, our analysis only covers radially symmetric potentials, yet.

We also show that the exponential decay of Bérenger solutions and the pole condition are almost equivalent. As a consequence, the class of applications of the PML method and methods based on the pole condition is almost the same. For a comparison of the numerical performance of both methods we refer to [6]. A potential advantage of methods based on the pole condition is the possibility to evaluate the exterior field numerically by a representation formula if the location and the type of the singularities in the Laplace domain are known. This is particularly relevant if a fundamental solution is not known explicitly. Otherwise, the exterior field can be evaluated by Green's representation formula.

The plan of this paper is as follows: In the next section we introduce the class of problems considered in this paper and the corresponding Dirichlet-to-Neumann map. In section 3 we prove the analytic continuation properties of the solution and review the correspondence to the pole condition. In section 4 a more detailed derivation of the PML equations is given. Finally, in the sections 5 and 6 we prove our main theorem on the exponential convergence of the solutions to the PML equations as $\rho \rightarrow \infty$.

2 Helmholtz scattering problem and the DtN Operator

We are concerned with Helmholtz-type scattering problems

$$\Delta u(x) + k^2(x) u(x) = 0 \text{ in } \mathbb{R}^d \setminus \Omega \quad (2.1a)$$

$$\frac{\partial}{\partial n} u|_{\partial K} = f \quad (2.1b)$$

$$\lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u}{\partial r} - i\kappa u \right) = 0. \quad (2.1c)$$

$K \subset \mathbb{R}^d$ denotes a compact smooth set and $f \in H^{-1/2}(\partial K)$. We assume that k is a bounded, continuous function which is given by

$$k^2(x) = (1 + p(|x|)) \kappa^2, \text{ for } |x| \geq a_*.$$

Here $p(t^{-1}) = \sum_{m=2}^{\infty} p_m t^m$ has a convergence radius greater than $\frac{1}{a_p}$, $a_p \in (0, \infty]$ with $a_* > a_p$. As proved in [4] the above system has a unique solution. We are only interested in the solution in the domain $\Omega_a = B_a^d \setminus \overline{K}$, where $a > a_*$. We denote $u^{(\text{int})}(x) = u(x)$, $x \in \Omega_a$. With the sesquilinear form $\mu : H^1(\Omega_a) \times H^1(\Omega_a) \rightarrow \mathbb{C}$,

$$\mu(u, v) := \int_{\Omega_a} \nabla u \nabla \bar{v} \, dx - \int_{\Omega_a} k^2 u \bar{v} \, dx - \int_{S_a^{d-1}} \text{DtN}_a u \bar{v} \, dS \quad (2.2)$$

and the continuous anti-linear functional $F : H^1(\Omega_a) \rightarrow \mathbb{C}$.

$$F(v) = \int_{\partial K} f \bar{v} \, dS \quad (2.3)$$

$u^{(\text{int})}$ is the unique solution to the variational problem

$$\mu(u, v) = F(v) \text{ for all } v \in H^1(\Omega_a),$$

(see [4]), which corresponds to the boundary value problem

$$\Delta u^{(\text{int})} + k^2 u^{(\text{int})} = 0 \text{ in } \Omega_a \quad (2.4a)$$

$$\partial_n u^{(\text{int})} = f \text{ on } \partial K \quad (2.4b)$$

$$\partial_r u^{(\text{int})} - \text{DtN}_a u^{(\text{int})} = 0 \text{ on } S_a^{d-1}. \quad (2.4c)$$

Here $S_a^{d-1} := \{x \in \mathbb{R}^d : |x| = a\}$. DtN_a denotes the *Dirichlet-to-Neumann map* $\text{DtN}_a : H^{1/2}(S_a^{d-1}) \rightarrow H^{-1/2}(S_a^{d-1})$, which is defined as follows. Given $g \in H^{1/2}(S_a^{d-1})$

$$\text{DtN}_a g = \partial_r u^{(\text{ext})}|_{S_a^{d-1}},$$

where $u^{(\text{ext})}$ is the unique solution to the exterior problem

$$\Delta u^{(\text{ext})} + k^2 u^{(\text{ext})} = 0 \text{ in } D_{a,\infty} \quad (2.5a)$$

$$u^{(\text{ext})}|_{\partial S_a^{d-1}} = g \quad (2.5b)$$

$$\lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u^{(\text{ext})}}{\partial r} - i\kappa u^{(\text{ext})} \right) = 0. \quad (2.5c)$$

Here and in the following we use the notations $D_{\theta_1, \theta_2} = B_{\theta_2}^d \setminus \overline{B_{\theta_1}^d}$, $D_{\theta_1, \infty} = \mathbb{R}^d \setminus \overline{B_{\theta_1}^d}$. We call the boundary condition (2.4c) transparent because it leads to the exact solution in the interior domain without any spurious reflections. It can be seen from the above definition of the DtN_a -operator the boundary condition (2.4c) is non-local. In particular, it is not given as a finite sum of differential operators acting on the boundary S_a^{d-1} . Moreover due to the inhomogeneous potential in the exterior domain the DtN_a -operator is not known explicitly as it is the case for constant potentials. Therefore with regard to a numerical approximation of the interior problem by the finite element method the use of the DtN_a -operator is not feasible. Nevertheless the DtN_a -operator will give us the theoretical framework to prove the convergence of the PML method. We will interpret the action of the sponge layer as a perturbation of the DtN_a -operator.

3 Analytic continuation of the exterior solution

We introduce polar coordinates $r > 0$ and $\hat{x} \in S_1^{d-1}$ in \mathbb{R}^d . With a slight misuse of notation, we use the same letter for exterior fields in polar and cartesian coordinates, i.e. $u(r, \hat{x}) = u(r\hat{x})$. If u is a solution to the boundary problem (2.5) we will show that $u(\cdot, \hat{x})$

has a holomorphic extension to $\mathbb{C}_a^{++} = \{z \in \mathbb{C} : \Re z > a, \Im z \geq 0\}$. Recall that the Laplace operator in polar coordinates is given by $\frac{1}{r^{d-1}} \partial_r (r^{d-1} \partial_r) + \frac{1}{r^2} \Delta_{\hat{x}}$, where $\Delta_{\hat{x}}$ denotes the Laplace-Beltrami operator on the unit sphere. We replace the real coordinate r by the complex variable z and define

$$\Delta_z = \frac{1}{z^{d-1}} \frac{\partial}{\partial z} z^{d-1} \frac{\partial}{\partial z} + \frac{1}{z^2} \Delta_{\hat{x}}.$$

As usual, we define $\frac{\partial}{\partial z} f(z) := \lim_{\bar{z} \in \mathbb{C}_a^{++} \rightarrow z} \frac{f(\bar{z}) - f(z)}{\bar{z} - z}$. Thus, ∂_z is a one sided derivative on the real axis. Later we will need the more general result that the boundary condition (2.5b) may be posed at a complex radius $z_0 \in \mathbb{C}_a^{++}$. In this case we seek a solution which is defined on $\mathbb{C}_{z_0}^{++} = \{z \in \mathbb{C} : \Re z > \Re a, \Im z \geq \Im z_0\}$. The next theorem is a generalization of [4, Theorem 24] for complex arguments. Since the proof is almost the same, it is omitted here.

Theorem 1 *Let $z_0 \in \mathbb{C}_a^{++}$ and $\tilde{g} \in H^{1/2}(S_1^{d-1})$ be given.*

1. *There exists a unique function $u \in C^2(\mathbb{C}_{z_0}^{++} \times S_1^{d-1})$, which is holomorphic in the first variable and satisfies*

$$\Delta_z u(z, \hat{x}) + k^2(z) u(z, \hat{x}) = 0, \quad z \in \mathbb{C}_{z_0}^{++}, \quad \hat{x} \in S_1^{d-1} \quad (3.1a)$$

$$u(z_0, \cdot) = \tilde{g} \quad (3.1b)$$

$$\lim_{\Re z \rightarrow \infty} z^{\frac{d-1}{2}} \left(\frac{\partial}{\partial z} u - i\kappa u \right) = 0. \quad (3.1c)$$

Condition (3.1b) has to be understood in the sense of the trace operator.

2. *There exist functions $u_\infty \in C^\infty(S_1^{d-1})$ and $\Psi \in C^1(\mathbb{R}_+ \times S_1^{d-1})$ and a constant $\tilde{a} > \Re z_0$ such that the above solution is given by*

$$u(z, \hat{x}) = z^{\frac{1-d}{2}} e^{i\kappa z} \left(u_\infty(\hat{x}) + \int_0^\infty e^{-t(z-\tilde{a})} \Psi(t, \hat{x}) dt \right) \quad (3.2)$$

for $\Re z \geq \tilde{a}$. $\Psi(t, \hat{x})$ decays exponentially as $t \rightarrow \infty$. The formula (3.2) may be differentiated any number of times both with respect to z and \hat{x} , integration and differentiation may be interchanged. Moreover, given $m \in \{0, 1\}$ and $l \in \{0, 1, \dots\}$, there exists a constant $C > 0$ such that

$$\|u_\infty\|_{C^l(S_1^{d-1})} \leq C \|\tilde{g}\|_{L^2}, \quad (3.3)$$

$$\int_0^\infty t^k \left\| \frac{\partial^m}{\partial t^m} \Psi(t, \cdot) \right\|_{C^l(S_1^{d-1})} dt \leq C \|\tilde{g}\|_{L^2}. \quad (3.4)$$

Let us consider the restriction $v(z) := u(z + a, \hat{x})$, $z \in \mathbb{C}_0^{++}$ of the solution to a ray with direction $\hat{x} \in S_1^{d-1}$. It follows from (3.2), (3.3) and (3.4) that

$$v \text{ has an holomorphic extension to } \mathbb{C}_0^{++} \quad (3.5a)$$

$$\sup_{z \in \mathbb{C}_0^{++}} |e^{-i\kappa z} v(z)| < \infty, \quad (3.5b)$$

i.e. that $v(z)$ decays exponentially as $\Im z \rightarrow \infty$. Since for an incoming wave $v(z)$ grows exponentially as $\Im z \rightarrow \infty$ (if the complex extension to $z \in \mathbb{C}_0^{++}$ exists at all), the exponential decay of $v(z)$ as $\Im z \rightarrow \infty$ characterizes outgoing waves. At the same time it is the foundation of the PML method, see e.g. [2]. We call the conditions (3.5) the PML condition.

The pole condition is an alternative characterization of outgoing waves, which is also the basis of numerical algorithms (cf. [6, 5]). For the differential equation (2.1a), (2.1c) we have shown in [4] that v satisfies the pole condition that is

$$\hat{v} \text{ has an holomorphic extension to } \{z \in \mathbb{C} : \Im z < \kappa\} \quad (3.6a)$$

$$\sup_{-\pi < \arg s < \pi/2} |s + i\kappa| |\hat{v}(s + i\kappa)| < \infty. \quad (3.6b)$$

For general differential equations, e.g. problems with waveguides, we do not have a proof that either (3.5) or (3.6) is an appropriate characterization of outgoing waves sufficient to show both existence and uniqueness of solutions. However, we will give an informal argument that if one of these conditions is satisfied, then both are satisfied. We have deliberately decided not to formulate this as a theorem as it would require many technical assumptions on v and \hat{v} which would conceal the main idea of the proof. For the differential equation (2.1a) all these assumptions are satisfied.

Assume that $v : [0, \infty) \rightarrow \mathbb{C}$ is a bounded analytic function, not necessarily related to the differential equation (2.1a), and that κ is a nonnegative real number. Note that the case $\kappa > 0$ can be reduced to the case $\kappa = 0$ by considering the function $w(z) = e^{-i\kappa z} v(z)$ with Laplace transform $\hat{w}(s) = \hat{v}(s + i\kappa)$.

We first assume that v satisfies (3.5) with $\kappa = 0$. Let $0 < \theta < \pi/2$ and $s \in \mathbb{C} \setminus \{0\}$ with $-\pi/2 < \arg s < \pi/2 - \theta$. Consider the contour in Figure 3.1a). By Cauchy's integral theorem, $\int_{\gamma_1^R + \gamma_2^R + \gamma_3^R} e^{-sz} v(z) dz = 0$ for all $R > 0$. Due to the boundedness of v , $\lim_{R \rightarrow \infty} \int_{\gamma_2^R} e^{-sz} v(z) dz =$

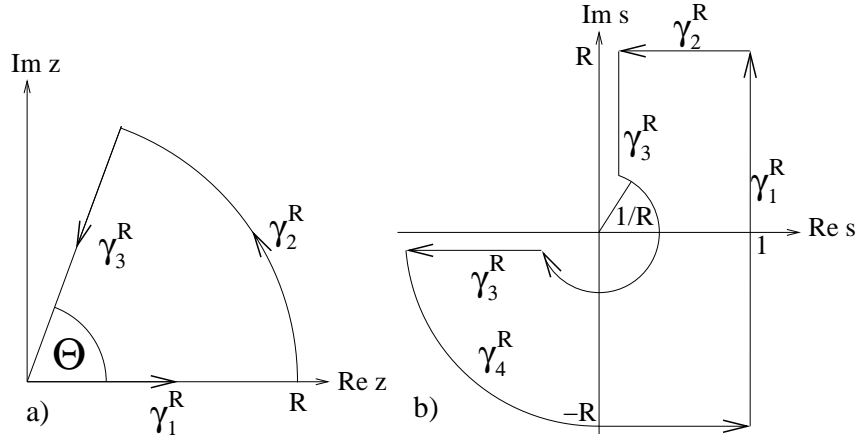


Fig. 3.1. Equivalence of the pole condition and the exponential decay of the Béranger functions

0. Therefore,

$$\begin{aligned}\hat{v}(s) &= \lim_{R \rightarrow \infty} \int_{\gamma_1^R} e^{-sz} v(z) dz \\ &= - \lim_{R \rightarrow \infty} \int_{\gamma_3^R} e^{-sz} v(z) dz = \int_0^{e^{i\theta} \infty} e^{-sz} v(z) dz.\end{aligned}$$

A partial integration yields

$$s\hat{v}(s) = v(0)e^{i\theta} + \int_0^{e^{i\theta} \infty} e^{-sz} v'(z) dz. \quad (3.7)$$

Using the estimate $|v'(z)| \leq \sup_{|\zeta-z|=\epsilon} \epsilon^{-1} |v(\zeta)|$ for holomorphic functions we can show that $\sup\{|v'(re^{i\theta})| : r \geq 0\} < \infty$. Then \hat{v} has a holomorphic extension to $\{s \in \mathbb{C} : \Re(se^{i\theta}) > 0\}$ and $\sup\{|sv(s)| : -\pi/2 + \delta < \arg(se^{i\theta}) < \pi/2 - \delta\} < \infty$ for any $\delta > 0$. Since θ can be chosen arbitrarily close to $\pi/2$, \hat{v} has a complex extension to $\{s \in \mathbb{C} : \Im s < 0\}$. To establish the uniform estimate (3.6b), we may either use an integro-differential equation for \hat{v} , or choose $\theta > \pi/2$ if that is possible.

Now assume that v satisfies (3.6) with $\kappa = 0$. Consider the contour in Figure 3.1b). By the Fourier inversion theorem we have

$$v(r) = \frac{1}{2\pi i} \lim_{R \rightarrow \infty} \int_{\gamma_1^R} e^{sr} \hat{v}(s) ds$$

for $r > 0$. Using (3.6b) it can be shown that $\lim_{R \rightarrow \infty} \int_{\gamma_2^R + \gamma_4^R} e^{sr} \hat{v}(s) \, ds = 0$. Hence, by Cauchy's integral theorem

$$v(z) = -\frac{1}{2\pi i} \lim_{R \rightarrow \infty} \int_{\gamma_3^R} e^{sz} \hat{v}(s) \, ds$$

for $z > 0$. If the limit above exists not only for $z > 0$, but also for $z \in \mathbb{C}_0^{++}$, we have obtained the desired extension of v to \mathbb{C}_0^{++} . Moreover, $|v(z)|$ is bounded at least for $\delta < \arg z < \pi/2 - \delta$, $\delta > 0$. Uniform boundedness of $|v|$ in all of \mathbb{C}_0^{++} can be shown if the integration paths can be tilted into the domain $\{s \in \mathbb{C} : \Re s < 0, \Im s > 0\}$. If other singularities of $\hat{v}(s)$ occur on the positive imaginary axis or the negative real axis, γ_3^R has to be deformed at these points as at $s = 0$.

4 The PML equation in the exterior domain

We assume that γ is of the form $\gamma(r) = r \left(1 + \frac{i}{r} \int_a^r \sigma(t) \, dt\right)$, where $\sigma \in C^1([a, \infty), \mathbb{R})$ satisfies

$$\sigma(a) = 0, \quad (4.1a)$$

$$\sup_{r \geq a} \sigma(r) < \infty, \quad (4.1b)$$

$$\lim_{r \rightarrow \infty} \inf_{r' \geq r} \sigma(r') > 0. \quad (4.1c)$$

The so called Bérenger function is defined by

$$u^{(B)}(r, \hat{x}) = u^{(\text{ext})}(\gamma(r), \hat{x}).$$

Observe that $u^{(B)}(a\hat{x}) = u^{(\text{ext})}(a\hat{x})$ and $\partial_r u^{(B)}(a\hat{x}) = \partial_r u^{(\text{ext})}(a\hat{x})$. Thus concerning the variational formulation of the inner domain problem, $u^{(B)}$ is as good as $u^{(\text{ext})}$. With this notation $u^{(B)}$ satisfies

$$\frac{1}{\gamma^{d-1} \gamma'} \frac{\partial}{\partial r} \left(\frac{\gamma^{d-1}}{\gamma'} \frac{\partial}{\partial r} u^{(B)} \right) + k^2(\gamma(r)) u^{(B)} + \frac{1}{\gamma^2} \Delta_{\hat{x}} u^{(B)} = 0. \quad (4.2)$$

In the next lemma we prove that $u^{(B)} \in H^1(\mathbb{R}^d \setminus \overline{B_a^d})$. We again allow a boundary condition (2.5b) at a complex radius $z_0 \in \mathbb{C}_a^{++}$.

Lemma 2 *Let $r_0 \geq a$. For $\tilde{g} \in H^{1/2}(S_1^{d-1})$ let u be the unique solution to (3.1) with $z_0 = \gamma(r_0)$. We write $u_\gamma(r, \hat{x}) := u(\gamma(r), \hat{x})$, $r \geq r_0$. Then $u_\gamma \in H^1(D_{r_0, \infty})$ and there exists a constant C independent of \tilde{g} such that $\|u_\gamma\|_{H^1} \leq C \|\tilde{g}\|_{H^{1/2}(S_1^{d-1})}$.*

Proof By Theorem 1, Part 2), there exist $\tilde{a} > a$ and a constant C such that $\|u_\gamma\|_{H^1(D_{\tilde{a},\infty})} \leq C \|\tilde{g}\|_{L^2}$. Therefore, it remains to show that $\|u_\gamma\|_{H^1(D_{r_0,\tilde{a}})} \leq C \|\tilde{g}\|_{H^{1/2}}$. For simplicity we assume $\kappa = 1$ here. Let $\{\varphi_j, \lambda_j : j \in \mathbb{N}\}$ be a complete orthonormal system of eigenfunctions and eigenvalues of the Laplace-Beltrami operator $\Delta_{\hat{x}}$ on the sphere S_1^{d-1} . We write $\tilde{g}_j = \int_{S_1^{d-1}} \tilde{g}(\cdot) \varphi_j dS$. By a generalization of [4, equation 35] we get the modal expansion of the solution $u(z, \hat{x})$ in $\mathbb{C}_{z_0}^{++}$

$$u(z, \hat{x}) = z_0^{\frac{d-1}{2}} z^{-\frac{d-1}{2}} \sum_{j=1}^{\infty} \tilde{g}_j \frac{\mathcal{H}_j(z)}{\mathcal{H}_j(z_0)} \varphi_j(\hat{x}). \quad (4.3)$$

The generalized Hankel functions \mathcal{H}_j are introduced in [4]. This yields

$$u_\gamma(r, \hat{x}) = z_0^{\frac{d-1}{2}} \sum_{j=1}^{\infty} \tilde{g}_j \gamma(r)^{-\frac{d-1}{2}} \frac{\mathcal{H}_j(\gamma(r))}{\mathcal{H}_j(z_0)} \varphi_j(\hat{x}). \quad (4.4)$$

We will show that this sum converges in $H^1(D_{r_0,\tilde{a}})$. By [4, Corollary 20] there exists a constant N such

$$\begin{aligned} \left| \frac{\mathcal{H}_j^{(l)}(\gamma(r))}{\mathcal{H}_j(z_0)} \right| &\leq C \left(\frac{\sqrt{-\lambda_j + \frac{(d-1)(d-3)}{4}}}{|\gamma(r)|} \right)^l \left| \frac{z_0}{\gamma(r)} \right|^{\sqrt{-\lambda_j + \frac{(d-1)(d-3)}{4}}} \\ &\leq C \left(\frac{\sqrt{-\lambda_j}}{|\gamma(r)|} \right)^l \left| \frac{z_0}{\gamma(r)} \right|^{\sqrt{-\lambda_j}} \\ &\leq C \left(\frac{\sqrt{-\lambda_j}}{|\gamma(r)|} \right) \left(\frac{r_0}{r} \right)^{\sqrt{-\lambda_j}} \end{aligned}$$

for all $j \geq N$, $r_0 \leq r \leq \tilde{a}$ and $l = 0, 1, 2$. Here and in the following C is a generic constant. Recall that the Sobolev norm of index $1/2$ on S_1^{d-1} is defined by

$$\|\tilde{g}\|_{H^{1/2}}^2 = \sum (1 + |\lambda_j|)^{1/2} |\tilde{g}_j|^2.$$

Let $M > N$ then

$$\begin{aligned}
& \left\| \gamma(r)^{-\frac{d-1}{2}} \sum_{j=1}^M f_j \frac{\mathcal{H}_j(\gamma(r))}{\mathcal{H}_j(z_0)} \varphi_j(\hat{x}) \right\|^2 \leq C \left\| \sum_{j=1}^M \tilde{g}_j \frac{\mathcal{H}_j(\gamma(r))}{\mathcal{H}_j(z_0)} \varphi_j(\hat{x}) \right\|^2 \\
& = C \sum_{j=1}^M \int_{r_0}^{\tilde{a}} r^{d-1} |\tilde{g}_j|^2 \left\{ \left| \frac{\mathcal{H}_j(\gamma(r))}{\mathcal{H}_j(z_0)} \right|^2 (1 + |\lambda_j|) + \left| \frac{\mathcal{H}_j^{(1)}(\gamma(r)) \gamma'(r)}{\mathcal{H}_j(z_0)} \right|^2 \right\} dt \\
& \leq C \|\tilde{g}\|_{L^2} + C \sum_{j=1}^{N-1} |\tilde{g}_j|^2 + C \sum_{j=N}^M |\tilde{g}_j|^2 (|\lambda_j|) \int_{r_0}^{\tilde{a}} \left(\frac{r_0}{r}\right)^{2\sqrt{-\lambda_j}} dr \\
& \leq C \|\tilde{g}\|_{L^2} + C \sum_{j=N}^M |\tilde{g}_j|^2 |\lambda_j|^{1/2}
\end{aligned}$$

where the generic constant C is independent of M . As $\|\tilde{g}\|_{H^{1/2}}^2 \leq C \sum_{j=1}^\infty (1 + |\lambda_j|^{1/2}) |\tilde{g}_j|^2$, we see that $\|u_\gamma\|_{H^1(D_{\Re z_0, \tilde{a}})} \leq C \|\tilde{g}\|_{H^{1/2}}$. \square

We will see that equation (4.2) has a quite simple form in cartesian coordinates.

Lemma 3 $u^{(B)} \in H^1(D_{a, \infty})$ satisfies the boundary value problem

$$\Delta_\gamma u + k_\gamma^2 u = 0 \quad (4.5a)$$

$$u|_{S_a^{d-1}} = g, \quad (4.5b)$$

where $k_\gamma^2(r) = k^2(\gamma(r))$ and Δ_γ has the form $\Delta_\gamma = \nabla \cdot A_\gamma \nabla + b_\gamma \nabla$ in cartesian coordinates. Here $A_\gamma \in C^1([a, \infty), \mathbb{C}^{d \times d})$ and $b_\gamma \in C^0([a, \infty), \mathbb{C}^{1 \times d})$ satisfy

$$A_\gamma(r, \hat{x}) = G_{\hat{x}}^T \text{diag} \left(\frac{1}{(\gamma'(r))^2}, \underbrace{\frac{r^2}{\gamma^2(r)}, \dots, \frac{r^2}{\gamma^2(r)}}_{(d-1) \times} \right) G_{\hat{x}}, \quad (4.6)$$

and

$$b_\gamma(r, \hat{x}) = \left(\frac{d-1}{r} - \frac{d-1}{\gamma(r) \gamma'(r)} - \frac{\gamma''(r)}{(\gamma'(r))^2}, \underbrace{0, \dots, 0}_{(d-1) \times} \right) G_{\hat{x}}$$

for an arbitrary orthogonal matrix $G_{\hat{x}}$ whose first line is \hat{x} .

Proof 1) For $u, v \in C_0^\infty(\mathbb{R}^d \setminus \bar{B}_a^d)$ we have

$$\begin{aligned} \int_{D_{a,\infty}} \Delta_\gamma u \bar{v} \, dx &= \int_a^\infty \int_{S^{d-1}} r^{d-1} \left[\frac{1}{\gamma^{d-1} \gamma'} \frac{\partial}{\partial r} \left(\frac{\gamma^{d-1}}{\gamma'} \frac{\partial}{\partial r} u \right) + \frac{1}{\gamma^2} \Delta_{\hat{x}} u \right] \bar{v} \, dr \, dS \\ &= - \int_a^\infty \int_{S^{d-1}} r^{d-1} \left[\frac{1}{(\gamma')^2} \frac{\partial}{\partial r} u \frac{\partial}{\partial r} \bar{v} + \frac{1}{\gamma^2} \nabla_{\hat{x}} u \cdot \nabla_{\hat{x}} \bar{v} \right] \bar{v} \, dr \, dS \\ &\quad - \int_a^\infty \int_{S^{d-1}} r^{d-1} \left[\left(\frac{d-1}{r} - \frac{d-1}{\gamma \gamma'} - \frac{\gamma''}{(\gamma')^3} \right) \frac{\partial}{\partial r} u \right] \bar{v} \, dx \end{aligned}$$

$\nabla_{\hat{x}}$ denotes the surface gradient on S_1^{d-1} . Recall that $\nabla_{\hat{x}} u(r, \hat{x})$ is the projection of $r \nabla u(r \hat{x})$ to the tangential plane, which is orthogonal to \hat{x} . Since this projection is given by $G_{\hat{x}}^T \text{diag}(0, 1, \dots, 1) G_{\hat{x}}$ we get

$$\nabla_{\hat{x}} u(r, \hat{x}) = r G_{\hat{x}}^T \text{diag}(0, 1, \dots, 1) G_{\hat{x}} \nabla u(r \hat{x}).$$

Analogously, $\hat{x} \frac{\partial}{\partial r} u(r, \hat{x}) = G_{\hat{x}}^T \text{diag}(1, 0, \dots, 0) G_{\hat{x}} \nabla u(r \hat{x})$. Therefore

$$\begin{aligned} \frac{\partial}{\partial r} u(r, \hat{x}) \frac{\partial}{\partial r} \overline{v(r, \hat{x})} &= (\nabla u(r \hat{x}))^T G_{\hat{x}}^T \text{diag}(1, 0, \dots, 0) G_{\hat{x}} \overline{\nabla v(r \hat{x})} \\ \nabla_{\hat{x}} u(r, \hat{x}) \cdot \nabla_{\hat{x}} \overline{v(r, \hat{x})} &= r^2 (\nabla u(r \hat{x}))^T G_{\hat{x}}^T \text{diag}(0, 1, \dots, 1) G_{\hat{x}} \overline{\nabla v(r \hat{x})}. \end{aligned}$$

Inserting this yields

$$\int_{D_{a,\infty}} \Delta_\gamma u \bar{v} \, dx = \int_{D_{a,\infty}} A_\gamma \nabla u \cdot \nabla \bar{v} + b_\gamma \nabla u \bar{v} \, dx$$

for all $v \in C_0^\infty(D_{a,\infty})$. This implies the asserted form of Δ_γ . To prove the regularity of A_γ and b_γ we may choose $G_{\hat{x}}$ such that it locally depends smoothly on \hat{x} . \square

Lemma 4 *The operator $\frac{\gamma \gamma'}{r} \Delta_\gamma$ is strongly elliptic on $D_{a,\infty}$.*

Proof By (4.6) we must show that there exists a $\delta > 0$ with

$$\max_{a \leq r < \infty} \left\{ \Re \frac{\gamma(r)}{r \gamma'(r)}, \Re \frac{r \gamma'(r)}{\gamma(r)} \right\} > \delta > 0.$$

But $\Re \left(\frac{\gamma}{r \gamma'} \right) = \frac{1 + \sigma \frac{1}{r} \int_a^r \sigma(t) \, dt}{1 + \sigma^2} \geq \frac{1}{1 + \max \sigma^2}$, $\Re \left(\frac{r \gamma'}{\gamma} \right) = \frac{1 + \sigma \frac{1}{r} \int_a^r \sigma(t) \, dt}{1 + \left(\frac{1}{r} \int_a^r \sigma(t) \, dt \right)^2} \geq \frac{1}{1 + \max \sigma^2}$. The assertion now follows from (4.1c). \square

In Lemma 8, Part 1) we prove that $u^{(B)}$ is the unique solution to (4.5) in $H^1(D_{a,\infty})$. So far, we have replaced the exterior Helmholtz

problem (2.5) by the Béranger problem (4.5), which is still posed on an unbounded domain. Motivated by the exponential decay of $u^{(B)}$ we restrict (4.5) onto a bounded domain, say $D_{a,\rho}$, $\rho > a$ and impose a zero Dirichlet boundary conditions on the artificial boundary S_ρ^{d-1} . This yields the so-called PML system

$$\Delta_\gamma u + k_\gamma^2 u = 0, \quad x \in D_{a,\rho} \quad (4.7a)$$

$$u|_{S_a^{d-1}} = g \quad (4.7b)$$

$$u|_{S_\rho^{d-1}} = 0. \quad (4.7c)$$

In the next sections we prove that this PML system has a unique solution $u_\rho^{(\text{PML})}$ for ρ large enough and suitable γ . Further we show that the perturbed Dirichlet -to-Neumann map $\text{DtN}_{a,\rho}^{(\text{PML})} : H^{1/2}(S_a^{d-1}) \rightarrow H^{-1/2}(S_a^{d-1})$ given by

$$g \mapsto \partial_r u_\rho^{(\text{PML})}$$

is well defined and converges exponentially fast to DtN_a as ρ tends to $+\infty$.

5 Exponential Convergence of $\text{DtN}_{a,\rho}^{(\text{PML})}$

In the following we are repeatedly concerned with boundary value problems of the type (4.5) and (4.7) on domains D_{θ_1,θ_2} , $\infty \geq \theta_2 > \theta_1 \geq a$. For a compact notation of these problems we make the following definitions.

Definition 5 *Let $\infty > \theta_2 > \theta_1 > a$ be given. We define the operators*

$$\mathcal{L}_{\theta_1,\theta_2} : H^1(D_{\theta_1,\theta_2}) \rightarrow H^{-1}(D_{\theta_1,\theta_2}) \times H^{1/2}(S_{\theta_1}^{d-1}) \times H^{1/2}(S_{\theta_2}^{d-1})$$

and

$$\mathcal{L}_{\theta_1,\infty} : H_{\text{loc}}^1(D_{\theta_1,\infty}) \rightarrow \mathcal{D}'(D_{\theta_1,\infty}) \times H^{1/2}(S_{\theta_1}^{d-1})$$

by $u \mapsto \left(\Delta_\gamma u + k_\gamma^2 u, u|_{S_{\theta_1}^{d-1}}, u|_{S_{\theta_2}^{d-1}} \right)$ and $u \mapsto \left(\Delta_\gamma u + k_\gamma^2 u, u|_{S_{\theta_1}^{d-1}} \right)$, respectively.

Remark 6 A function $u \in H^1(D_{a,\infty})$ solves the Béranger system (4.5) if and only if it satisfies $\mathcal{L}_{a,\infty} u = (0, g)$. A function $u \in H^1(D_{a,\rho})$ solves the PML system (4.7) if and only if it satisfies $\mathcal{L}_{a,\rho} u = (0, g, 0)$.

For the proof of the following lemma we restrict the class of admissible paths γ by the following conditions: There exist $a' > a, \sigma_0 > 0$ and $\epsilon > 0$ such that

$$\gamma(r) = (1 + i\sigma_0)r \quad (5.1a)$$

and

$$\kappa^2 \alpha_0^2 \sum_{m=2}^{\infty} \left| \frac{p_m}{\alpha_0^m r^m} \right| < \frac{\min(1, \kappa^2) \sigma_0}{|\alpha_0|} \quad (5.1b)$$

for $r \geq a'$ with $\alpha_0 := (1 + i\sigma_0)$. For simplicity we assume $a' \geq 1$.

Remark 7 *The condition (5.1a) means that γ is a straight line in the complex plane for $r \geq a'$. It is easily checked that $\Delta_\gamma = \frac{1}{\alpha_0^2} \Delta$ for $r \geq a'$. Therefore (4.5a) is equivalent to*

$$(\Delta + \alpha_0^2 k^2 (\alpha_0 |x|)) u^{(B)} = 0, \quad |x| > a'$$

which means that $u^{(B)}$ satisfies a Helmholtz equation with a complex wave number for $|x| > a'$.

Lemma 8 *The following holds true:*

1. For $\theta \geq a$ the operator $\mathcal{L}_{\theta, \infty}^{-1}$ is well defined and bounded from $\{0\} \times H^{1/2}(S_\theta^{d-1})$ to $H^1(D_{\theta, \infty})$.
2. The operator $\mathcal{L}_{a', \rho}$ has a bounded inverse for $\rho > a' + 1$, where a' is defined in (5.1). There exists a constant C such that $\|\mathcal{L}_{a', \rho}^{-1}\| \leq C\rho$ for all $\rho > a' + 1$.
3. $\mathcal{L}_{\theta_1, \theta_2}$ is a Fredholm operator with index zero.

Proof (1) Let $g \in H^{1/2}(S_\theta^{d-1})$ and let u denote the unique solution to (3.1) with $z_0 = \gamma(\theta)$ and $\tilde{g}(\hat{x}) = g(\theta\hat{x})$ in Theorem 1. Then $u_\gamma \in H^1(D_{\theta, \infty})$ given in Lemma 2 solves $\mathcal{L}u_\gamma = (0, g)$, and there exists a constant C such that $\|u_\gamma\| \leq C\|g\|$. Uniqueness is shown by a mode-wise argument as in [4].

(2) Given $(f, h_{a'}, h_\rho) \in H^{-1}(D_{a', \rho}) \times H^{1/2}(S_{a'}^{d-1}) \times H^{1/2}(S_\rho^{d-1})$ we must show that the equation

$$\mathcal{L}_{a', \rho} u = (f, h_{a'}, h_\rho) \quad (5.2)$$

has a unique solution $u \in H^1(D_{a',\rho})$ and that $\|u\| \leq C\rho\|(f, h_{a'}, h_\rho)\|$. By Remark 7, equation (5.2) is equivalent to

$$\tilde{\mathcal{L}}u = \alpha_0^2 f \quad (5.3a)$$

$$u|_{S_{a'}^d} = h_{a'} \quad (5.3b)$$

$$u|_{S_\rho^d} = h_\rho \quad (5.3c)$$

with the operator $\tilde{\mathcal{L}} : H^1(D_{a',\rho}) \rightarrow H^{-1}(D_{a,\rho})$ given by

$$u \mapsto \left[\Delta + \left(1 + \sum_{m=2}^{\infty} \frac{p_m}{\alpha_0^m |x|^m} \right) \kappa^2 \alpha_0^2 \right] u.$$

It is obvious that there exists a constant C_1 independent of ρ such that $\|\tilde{\mathcal{L}}\| \leq C_1$. Select a right inverse $R_{1,2}$ of the trace mapping $H^1(D_{1,2}) \rightarrow H^{1/2}(S_1^{d-1}) \times H^{1/2}(S_2^{d-1})$, $u \mapsto (u|_{S_1^{d-1}}, u|_{S_2^{d-1}})$. Using $R_{1,2}$ we define a right inverse of the trace mapping $H^1(D_{a',\rho}) \rightarrow H^{1/2}(S_{a'}^{d-1}) \times H^{1/2}(S_\rho^{d-1})$, $u \mapsto (u|_{S_{a'}^{d-1}}, u|_{S_\rho^{d-1}})$ by

$$R_{a',\rho}(h_{a'}, h_\rho)(r\hat{x}) := [R_{1,2}(h_{a'}(a'\cdot), h_\rho(\rho/2\cdot))] \left(\frac{\rho + r - 2a'}{\rho - a'} \hat{x} \right).$$

Recall that $a' \geq 1$, $\rho \geq 2$ and that

$$\|f\|_{H^{1/2}(S_\theta^{d-1})} = \theta^{(d-1)/2} \left\| (1 - \theta^{-2} \Delta_{\hat{x}})^{1/4} f(\theta^{-1}\cdot) \right\|_{L^2(S_1^{d-1})}.$$

Now,

$$\begin{aligned} & \|R_{a',\rho}(h_{a'}, h_\rho)\| \\ & \leq C\rho^{d/2} \max \left\{ \|h_{a'}(a'\cdot)\|_{H^{1/2}(S_1^{d-1})}, \|h_\rho(\rho/2\cdot)\|_{H^{1/2}(S_2^{d-1})} \right\} \\ & \leq C\rho^{d/2} \max \left\{ \frac{(a')^{1/2}}{(a')^{(d-1)/2}} \|h_{a'}\|_{H^{1/2}(S_{a'}^{d-1})}, \right. \\ & \quad \left. \frac{2^{(d-1)/2}}{\rho^{(d-1)/2}} \left(\frac{\rho^2}{4} \right)^{1/4} \|h_\rho\|_{H^{1/2}(S_\rho^{d-1})} \right\} \\ & \leq C_2\rho \max \left\{ \|h_{a'}\|_{H^{1/2}(S_{a'}^{d-1})}, \|h_\rho\|_{H^{1/2}(S_\rho^{d-1})} \right\} \end{aligned}$$

with a constant C_2 independent of ρ . Therefore, $\|R_{a',\rho}\| \leq C_2\rho$. Let $\mathcal{A} : H_0^1(D_{a',\rho}) \rightarrow H_0^1(D_{a',\rho})$ and $\mathcal{P} : H_0^1(D_{a',\rho}) \rightarrow H_0^1(D_{a',\rho})$ be the

operators defined by

$$\begin{aligned} \langle (\Delta w + \kappa^2 \alpha_0^2 w), \bar{v} \rangle &= (\mathcal{A}w, v) \\ \left\langle \kappa^2 \alpha_0^2 \sum_{m=2}^{\infty} \frac{p_m}{\alpha_0^m |x|^m} w, \bar{v} \right\rangle &= (\mathcal{P}w, v) \end{aligned}$$

for all $w, v \in H_0^1(D_{a',\rho})$. u solves (5.3) if and only if $w := u - R_{a',\rho}(h_{a'}, h_\rho)$ satisfies

$$(\mathcal{A} + \mathcal{P})w = \alpha_0^2 \mathcal{J}f - \mathcal{J}\tilde{\mathcal{L}}R_{a',\rho}(h_{a'}, h_\rho)$$

where \mathcal{J} denotes the canonical isomorphism between $H^{-1}(D_{a',\rho})$ and $H^1(D_{a',\rho})$. Obviously, $\|\mathcal{A}\|, \|\mathcal{P}\| \leq C_3$ with a constant C_3 independent of ρ . Since $\Im(\alpha_0) = \sigma_0 > 0$, the invertibility of \mathcal{A} follows by standard arguments. Further we have

$$\Im\left(\frac{1}{\alpha_0} \mathcal{A}u, u\right) = \frac{\sigma_0}{1 + \sigma_0^2} \langle \nabla u, \overline{\nabla u} \rangle + \kappa^2 \sigma_0 \langle u, \bar{u} \rangle.$$

Therefore

$$\frac{\min(1, \kappa^2) \sigma_0}{1 + \sigma_0^2} (u, u) \leq \Im\left(\frac{1}{\alpha_0} \mathcal{A}u, u\right) \leq \frac{1}{|\alpha_0|} \|\mathcal{A}u\| \|u\|$$

which yields $\|\mathcal{A}^{-1}\| \leq \frac{|\alpha_0|}{\min(1, \kappa^2) \sigma_0}$. By assumption (5.1b)

$$\begin{aligned} |(\mathcal{P}u, v)| &\leq \max_{r \in [a', \rho]} |\kappa^2 \alpha_0^2 p(\alpha_0 r)| \int_{B_\rho^d \setminus B_{a'}^d} |u \bar{v}| dx \\ &< \left(\frac{\min(1, \kappa^2) \sigma_0}{|\alpha_0|} \right) \|u\|_{L^2} \|v\|_{L^2} \end{aligned}$$

so $\|\mathcal{P}\| < \frac{\min(1, \kappa^2) \sigma_0}{|\alpha_0|}$. This implies $\|\mathcal{A}^{-1} \mathcal{P}\| \leq C_4 < 1$ with a constant C_4 independent of ρ . Hence $\mathcal{A} + \mathcal{P} = \mathcal{A}(I + \mathcal{A}^{-1} \mathcal{P})$ is invertible and $\|(\mathcal{A} + \mathcal{P})^{-1}\| \leq \frac{C_3}{1 - C_4}$. The estimate

$$\begin{aligned} \|u\| &= \left\| (\mathcal{A} + \mathcal{P})^{-1} \mathcal{J} \left(\alpha_0^2 f - \tilde{\mathcal{L}}R_{a',\rho}(h_{a'}, h_\rho) \right) + R_{a',\rho}(h_{a'}, h_\rho) \right\| \\ &\leq \frac{C_3}{1 - C_4} |\alpha_0^2| \|f\| + \left(\frac{C_3 C_1}{1 - C_4} + 1 \right) C_2 \rho \|(h_{a'}, h_\rho)\| \end{aligned}$$

completes the proof.

(3) We use Theorem 13.4 in [12]. The case $d > 2$ is clear. For $d = 2$ we must show that Δ_γ is properly elliptic. By the definitions 10.5.2

and 10.5.3 in [12] and 4.6 it suffices to show that the polynomial $P(z) = \frac{1}{(\gamma'(r))^2} + z^2 \frac{r^2}{\gamma^2(r)}$ has one root with $\Im z > 0$ and one root with $\Im z < 0$. The roots are given by $z_{\pm} = i \frac{\gamma(r)}{r\gamma'(r)}$. Since $\Re\left(\frac{\gamma}{r\gamma'}\right) = \frac{1+\sigma \frac{1}{r} \int_a^r \sigma(t) dt}{1+\sigma^2} \geq \frac{1}{1+\max \sigma^2}$ the assertion follows from (4.1c). \square

We emphasize that in the previous lemma we did not prove the solvability of the PML system (4.7) or equivalently the solvability of $\mathcal{L}_{a,\rho} u = (0, g, 0)$. This will be done in the following for ρ large enough by a technique proposed by Lassas and Somersalo in [8]. The key idea is to introduce propagation operators which allows an equivalent formulation of the Béranger and the PML problem on a fixed domain. Then the PML problem can be interpreted as a perturbed Béranger problem.

Definition 9 For $a' < \theta_1 \leq \theta_2$ we define the propagation operators $P_{\theta_1}^{(\theta_2)}, P_{\theta_1}^{(\infty)} : H^{1/2}(S_{a'}^{d-1}) \rightarrow H^{1/2}(S_{\theta_1}^{d-1})$ by

$$P_{\theta_1}^{(\theta_2)} h = \mathcal{L}_{a',\theta_2}^{-1}(0, h, 0)|_{S_{\theta_1}^{d-1}}$$

and

$$P_{\theta_1}^{(\infty)} h = \mathcal{L}_{a',\infty}^{-1}(0, h)|_{S_{\theta_1}^{d-1}}.$$

Lemma 10 1. The restriction of $u^{(B)}$ to $D_{a,a''}$ is the unique solution in $u \in H^1(D_{a,a''})$ to the equation

$$\mathcal{L}_{a,a''} u = \left(0, g, P_{a''}^{(\infty)}(u|_{S_{a'}^{d-1}})\right). \quad (5.4)$$

2. Let $u \in H^1(D_{a,\rho})$ satisfies (4.7a) Then u satisfies (4.7b) and (4.7c) if and only if

$$\mathcal{L}_{a,a''} u|_{D_{a,a''}} = \left(0, g, P_{a''}^{(\rho)}(u|_{S_{a'}^{d-1}})\right). \quad (5.5)$$

Proof 1) $u^{(B)}$ satisfies (5.4) by construction. Let u be any solution of (5.4) and $w = \mathcal{L}_{a',\infty}^{-1}(u|_{S_{a'}^{d-1}})$. Then $w|_{S_{a'}^{d-1}} = u|_{S_{a'}^{d-1}}$ and $w|_{S_{a''}^{d-1}} = u|_{S_{a''}^{d-1}}$. Hence we conclude that $w = u = \mathcal{L}_{a',a''}^{-1}(0, w|_{S_{a'}^{d-1}}, w|_{S_{a''}^{d-1}})$ in $B_{a''} \setminus \bar{B}_{a'}$. Therefore, the function

$$W(x) = \begin{cases} u(x), & x \in B_{a''}^d \setminus \overline{B_a^d} \\ w(x), & x \in \mathbb{R}^d \setminus B_{a''}^d \end{cases}$$

solves $\mathcal{L}_{a,\infty}W = (0, g)$. Hence $W = u^{(B)}$, and in particular $u = u^{(B)}|_{B_{a''} \setminus \overline{B_a^d}}$.

(2) Any solution u to (4.7) solves (5.5) by construction. Conversely, let $u \in H^1(D_{a,\rho})$ satisfy (4.7a) and (5.5) and let $w = \mathcal{L}_{a',\rho}^{-1}(0, u|_{S_{a'}^{d-1}}, 0)$. Then $w|_{S_{a'}^{d-1}} = u|_{S_{a'}^{d-1}}$ and $w|_{S_{a''}^{d-1}} = u|_{S_{a''}^{d-1}}$, and by virtue of Lemma 8 (2) $u(x) = w(x)$ for $x \in B_{a''}^d \setminus B_{a'}^d$. By the unique continuation principle for elliptic equations (see [3, Section 8.3]) we conclude that $u(x) = w(x)$ for $x \in B_\rho^d \setminus B_{a'}^d$. In particular u satisfies (4.7c). (4.7b) is an immediate consequence of (5.5). \square

Again, we did not prove that equation (5.5) has a solution.

Lemma 11 *Let $a' < a'' < \infty$. The following holds true:*

1. $P_{a''}^{(\infty)}$ is a compact operator.
2. There exists a constant C such that for all $\rho > a''$ and all $h \in H^{1/2}(S^{d-1}a')$

$$\left\| P_\rho^{(\infty)} h \right\|_{H^{1/2}} \leq C e^{-\kappa \sigma_0 \rho} \|h\|_{H^{1/2}}. \quad (5.6)$$

3. There exists a constant C such that for all $\rho > a''$

$$\left\| P_{a''}^{(\infty)} - P_{a''}^{(\rho)} \right\| \leq C \rho e^{-\kappa \sigma_0 \rho}. \quad (5.7)$$

Proof (1) We use the same notation as in the proof of Lemma (2). By (4.4) we have

$$P_{a''}^{(\infty)} h = r^{-\frac{d-1}{2}} (a')^{\frac{d-1}{2}} \sum_{j=1}^{\infty} \underbrace{\tilde{h}_j \frac{\mathcal{H}_j(\alpha_0 a'')}{\mathcal{H}_j(\alpha_0 a')}}_{\tilde{H}_j} \varphi_j(\hat{x})$$

with $\tilde{h}_j = \int_{S_1^{d-1}} h(a' \hat{x}) \varphi_j(\hat{x}) \, d\hat{x}$. By [4, Corollary 20] it holds true that

$$\left| \tilde{H}_j \right| \leq C \left| \tilde{h}_j \right| \left(\frac{a'}{a''} \right)^{\sqrt{-\lambda_j + \frac{(d-1)(d-3)}{4}}} \leq C \left| \tilde{h}_j \right| \left(\frac{a'}{a''} \right)^{\sqrt{-\lambda_j}}$$

with a generic constant C . Define the operators $P_N : H^{1/2}(S_{a'}^{d-1}) \rightarrow H^{1/2}(S_{a''}^{d-1})$ by

$$h \mapsto r^{-\frac{d-1}{2}} (a')^{\frac{d-1}{2}} \sum_{j=1}^N \tilde{H}_j \varphi_j(\hat{x}).$$

Obviously, P_N has finite rank and is therefore compact. Further,

$$\left\| P_{a''}^{(\infty)} h - P_N h \right\| = C \max_{j > N} \left\{ \left(\frac{a'}{a''} \right)^{\sqrt{-\lambda_j}} \right\} \|h\|.$$

Since $-\lambda_j \rightarrow \infty$ we conclude that P_N converge to $P_{a''}^{(\infty)}$. Therefore, $P_{a''}^{(\infty)}$ is also a compact operator, cf. [9, Theorem 1.4.3].

(2) Let $h \in H^{1/2}(S_{a'}^{d-1})$ be given and let u denote the unique solution to (3.1) with $z_0 = \gamma(a') = (1 + i\sigma_0)r$ and $\tilde{g}(\hat{x}) = h(a'\hat{x})$. By Theorem 1, Part 2) we have

$$\begin{aligned} (\mathcal{L}_{\rho, \infty}^{-1}(0, h))(r\hat{x}) &= [(1 + i\sigma_0)r]^{(1-d)/2} e^{i\kappa r} e^{-\kappa\sigma_0 r} \\ &\quad \left(u_\infty(\hat{x}) + \int_0^\infty e^{-t((1+i\sigma_0)r - \tilde{a})} \Psi(t, \hat{x}) dt \right). \end{aligned}$$

Further by the estimates (3.3) and (3.4) there exists a constant C such that for all $z \in \mathbb{C}_{z_0}^{++}$

$$\|u_\infty\|_{H^{1/2}(S_1^{d-1})}, \left\| \int_0^\infty e^{-t(z - \tilde{a})} \Psi(t, \cdot) dt \right\|_{H^{1/2}(S_1^{d-1})} \leq C \|\tilde{g}\|_{L^2(S_1^{d-1})}.$$

Using

$$\|f\|_{H^{1/2}(S_\rho^{d-1})} = \rho^{(d-1)/2} \left\| (1 - \rho^{-2} \Delta_{\hat{x}})^{1/4} f(\rho^{-1} \cdot) \right\|_{L^2(S_1^{d-1})}$$

we get

$$\begin{aligned} \left\| \mathcal{L}_{a', \infty}^{-1}(0, h) \right\|_{S_\rho^{d-1}} &\leq C e^{-\kappa\sigma_0\rho} \|\tilde{g}\|_{L^2(S_1^{d-1})} \\ &\leq C e^{-\kappa\sigma_0\rho} \|h\|_{H^{1/2}(S_{a'}^{d-1})}. \end{aligned}$$

Since $P_\rho^\infty = \mathcal{L}_{a', \infty}^{-1}(0, h)|_{S_\rho^{d-1}}$, this yields (5.6).

(3) Let $h \in H^{1/2}(S_{a'}^{d-1})$ be given. By the definition of $P_{a''}^{(\infty)}$ and $P_{a''}^{(\rho)}$ we have $P_{a''}^{(\infty)} h - P_{a''}^{(\rho)} h = \text{Tr}_{S_{a''}^{d-1}} \mathcal{L}_{a', \rho}^{-1}(0, 0, P_\rho^{(\infty)} h)$. Using Lemma 8, Part 2) and (5.6) we obtain

$$\left\| P_{a''}^{(\infty)} h - P_{a''}^{(\rho)} h \right\|_{H^{1/2}} = \left\| \text{Tr}_{S_{a''}^{d-1}} \right\| \left\| \mathcal{L}_{a', \rho}^{-1} \right\| \left\| P_\rho^{(\infty)} h \right\| \leq C \rho e^{-\kappa\sigma_0\rho} \|h\|,$$

which yields (5.7). \square

Proposition 12 *There exists a constant $\rho_0^{(\text{ext})} > a$ such that (4.7) has a unique solution for $\rho \geq \rho_0^{(\text{ext})}$. The operator $\text{DtN}_{a,\rho}^{(\text{PML})}$ is well defined for $\rho \geq \rho_0^{(\text{ext})}$, and there exists a constant C such that*

$$\left\| \text{DtN}_a - \text{DtN}_{a,\rho}^{(\text{PML})} \right\| \leq C e^{-\kappa \sigma_0 \rho}. \quad (5.8)$$

Here we use the operator norm of $L(H^{1/2}(S_a^{d-1}), H^{-1/2}(S_a^{d-1}))$.

Proof Define the operator $\mathcal{K} : H^1(B_{a''}^d \setminus \overline{B_a^d}) \rightarrow H^{-1}(B_{a''}^d \setminus B_a^d) \times H^{1/2}(S_a^{d-1}) \times H^{1/2}(S_{a'}^{d-1})$ by $u \mapsto (0, 0, P_{a''}^{(\infty)} u|_{S_{a'}^{d-1}})$. By Lemma 10, Part 1) $u^{(\text{B})}$ satisfies

$$\mathcal{L}_{a,a''} u^{(\text{B})} - \mathcal{K} u^{(\text{B})} = (0, g, 0). \quad (5.9)$$

The operator $\mathcal{L}_{a,a''}$ is of Fredholm index zero and \mathcal{K} is compact by Proposition 11, Part 1). Hence, $\mathcal{L}_{a,a''} - \mathcal{K}$ also has Fredholm index zero. To prove injectivity, assume u_0 satisfies (5.9) with $g = 0$. Then $\mathcal{L}_{a,a''} u_0 = (0, 0, P_{a''}^{(\infty)} u|_{S_{a'}^{d-1}})$ and hence by Lemma 10, Part 1) $u_0 = \mathcal{L}_{a,\infty}^{-1}(0, 0) = 0$. Thus, $(\mathcal{L}_{a,a''} - \mathcal{K})^{-1}$ exists. Next, consider the system (5.5). The same argument as above yields an equation

$$(\mathcal{L}_{a,a''} - \tilde{\mathcal{K}}) u_\rho^{(\text{PML})} = (0, g, 0) \quad (5.10)$$

with $\tilde{\mathcal{K}} u = (0, 0, P_{a'',\rho} \text{Tr}_{a'})$. Applying $(\mathcal{L}_{a,a''} - \mathcal{K})^{-1}$ on both sides of (5.10) yields

$$(I + (\mathcal{K} - \tilde{\mathcal{K}})) u_\rho^{(\text{PML})} = u^{(\text{B})}. \quad (5.11)$$

As $(\mathcal{K} - \tilde{\mathcal{K}}) u = (0, 0, (P_{a''}^{(\infty)} - P_{a''}^{(\rho)}) \text{Tr}_{a'})$ it follows from Proposition 11, Part 3) that $\|\mathcal{K} - \tilde{\mathcal{K}}\| \leq C \rho e^{-\kappa \sigma_0 \rho}$. Therefore (5.11) is solvable by a Neumann series for ρ large enough and we conclude that

$$\begin{aligned} \|u^{(\text{B})} - u_\rho^{(\text{PML})}\|_{H^1(D_{a,a''})} &\leq \frac{C \rho e^{-\kappa \sigma_0 \rho}}{1 - C \rho e^{-\kappa \sigma_0 \rho}} \|u^{(\text{B})}\| \\ &\leq C \rho e^{-\kappa \sigma_0 \rho} \|g\|. \end{aligned}$$

We claim that any $u \in H^1(D_{a,a''})$ satisfying $\nabla \cdot A_\gamma \nabla u + b_\gamma \nabla u + k_\gamma^2 u = 0$ has a normal derivative $\partial_r u|_{S_a^{d-1}} \in H^{-1/2}(S_a^{d-1})$, which satisfies $\|\partial_r u|_{S_a^{d-1}}\|_{H^{-1/2}} \leq C \|u\|_{H^1}$ with some constant $C > 0$. To see this

we choose a right inverse $R_a : H^{1/2}(S_a^{d-1}) \rightarrow H^1(D_{a,a''})$ of the trace operator $\varphi \mapsto \varphi|_{S_a^{d-1}}$ satisfying $\text{supp} R_a \varphi \subset D_{a, \frac{a+a''}{2}}$ for all $\varphi \in H^{1/2}(S_a^{d-1})$. Given $\varphi \in H^{1/2}(S_a^{d-1})$, we multiply the differential equation by $R_a \varphi$, integrate and formally use the Gauss divergence theorem and the identity $A_\gamma(a, \hat{x}) = Id$ to obtain

$$\left\langle \partial_r u|_{S_a^{d-1}}, \varphi \right\rangle = \int_{D_{a,\rho}} -A_\gamma \nabla u \cdot \overline{\nabla R_a \varphi} + b_\gamma \cdot \nabla u \overline{R_a \varphi} + k_\gamma^2 u R_a \varphi \, dx.$$

Since the right hand side of this equation is bounded by

$$\max \left\{ \|A_\gamma\|_\infty, \|b_\gamma\|_\infty, \|k_\gamma^2\|_\infty \right\} \|u\|_{H^1} \|R_a \varphi\|_{H^{1/2}},$$

we have proved the existence of $\partial_r u \in H^{-1/2}(S_a^{d-1})$ and the asserted bound. Putting everything together, we obtain the desired estimate

$$\begin{aligned} \left\| \text{DtN}_a g - \text{DtN}_a^{(\text{PML})} g \right\| &\leq C \left\| u_\rho^{(\text{PML})} - u^{(\text{B})} \right\|_{H^1(D_{a,a''})} \\ &\leq C \rho e^{-\kappa \sigma_0 \rho} \|g\|. \end{aligned}$$

□

6 Convergence of the PML solution in the interior domain

So far we have only considered the PML equation in the exterior domain. We will now derive the complete PML system in variational form on $B_\rho^d \setminus \overline{K}$ and show the convergence of the PML-solution in the interior domain Ω_a . We introduce the Hilbert space $H_{(0)}^1(\Omega_\rho) := \left\{ v \in H^1(\Omega_\rho) : v|_{S_\rho^{d-1}} = 0 \right\}$. We extend A_γ , b_γ and k_γ to Ω_a by Id , $[0, \dots, 0]$ and k^2 , respectively and define $\mu_\rho^{(\text{PML})} : H_{(0)}^1(\Omega_\rho) \times \underbrace{H_{(0)}^1(\Omega_\rho)}_{d \times} \rightarrow \mathbb{C}$ by

$$\mu_\rho^{(\text{PML})}(u, v) = \int_{\Omega_\rho} (A_\gamma \nabla u) \cdot \overline{\nabla v} + b_\gamma \cdot \nabla u \overline{v} + k_{\text{PML}}^2 u \overline{v} \, dx.$$

The functional F is defined in equation (2.3).

Theorem 13 *There exists a constant $\rho_0 \geq \rho_0^{(\text{ext})}$ and C such that the variational problem*

$$\mu_\rho^{(\text{PML})}(u, v) = F(v) \text{ for all } v \in H_{(0)}^1(\Omega_\rho) \quad (6.1)$$

has a unique solution $u_\rho^{(\text{PML})}$ for $\rho \geq \rho_0$. Further, for $\rho \geq \rho_0$

$$\left\| u^{(\text{B})} - u_\rho^{(\text{PML})} \right\|_{H^1(\Omega_a)} \leq C \rho e^{-\kappa \sigma_0 \rho} \quad (6.2)$$

with a constant C independent of ρ .

Before proving this theorem we need the following lemma, in which the error introduced by a perturbed DtN_a-operator is estimated.

Lemma 14 *Let $\widetilde{\text{DtN}}_a \in L(H^{1/2}(S_a^{d-1}), H^{-1/2}(S_a^{d-1}))$. There exist constants $\epsilon_0, C > 0$ such that*

$$\left\| \widetilde{\text{DtN}}_a - \text{DtN}_a \right\| \leq \epsilon_0$$

implies the existence and uniqueness of a solution $\widetilde{u}_{\text{int}} \in H^1(B_a^d \setminus \overline{\Omega})$ to the system (2.4) with DtN_a replaced by $\widetilde{\text{DtN}}_a$. Moreover,

$$\left\| \widetilde{u}^{(\text{int})} - u^{(\text{int})} \right\| \leq C \left\| \widetilde{\text{DtN}}_a - \text{DtN}_a \right\|. \quad (6.3)$$

Proof Let us define $\mathcal{A}, \mathcal{B} : H^1(\Omega_a) \rightarrow H^1(\Omega_a)$ and $\mathcal{G}, \mathcal{S} \in H^{-1}(\Omega_a)$ by

$$\begin{aligned} \langle \nabla u, \nabla \bar{v} \rangle - \langle k^2 u, \bar{v} \rangle - \int_{S_a^{d-1}} \text{DtN}_a u \bar{v} \, ds &= (\mathcal{A}u, v) \\ \int_{S_a^{d-1}} \text{DtN}_a u \bar{v} \, ds &= (\mathcal{B}u, v) \\ \int_{\partial\Omega} g \bar{v} \, ds &= (\mathcal{G}, v) \\ \int_{S_a^{d-1}} \text{DtN}_a u^{(\text{src})} \bar{v} \, ds &= (\mathcal{S}, v) \end{aligned}$$

for all $v \in H^1(B_a^d \setminus \overline{\Omega})$. $\widetilde{\mathcal{B}}$ and $\widetilde{\mathcal{S}}$ are defined analogously, where DtN_a is replaced by $\widetilde{\text{DtN}}_a$. As proved in [4] \mathcal{A}^{-1} exists and hence $u^{(\text{int})} = \mathcal{A}^{-1}(\mathcal{G} + \mathcal{S})$. To prove existence and uniqueness of $\widetilde{u}^{(\text{int})}$ for a given $\widetilde{\text{DtN}}_a$ we must show that $(\mathcal{A} + \mathcal{B} - \widetilde{\mathcal{B}})^{-1}$ exists and is bounded. Observe that

$$\begin{aligned} \left| \left((\mathcal{B} - \widetilde{\mathcal{B}}) u, v \right) \right| &= \left| \int_{S_a^{d-1}} (\text{DtN}_a u - \widetilde{\text{DtN}}_a u) \bar{v} \, ds \right| \\ &\leq \left\| \text{DtN}_a - \widetilde{\text{DtN}}_a \right\| \left\| u|_{S_a^{d-1}} \right\|_{H^{1/2}} \left\| v|_{S_a^{d-1}} \right\|_{H^{1/2}} \\ &\leq c \left\| \text{DtN}_a - \widetilde{\text{DtN}}_a \right\| \|u\| \|v\|. \end{aligned}$$

Hence $\|B - \tilde{B}\| \leq c \|\text{DtN}_a - \widetilde{\text{DtN}_a}\|$. The existence of

$$(\mathcal{A} + B - \tilde{B})^{-1} = \left(\mathcal{A} \left[I + \mathcal{A}^{-1} (B - \tilde{B}) \right] \right)^{-1}$$

for $\|\text{DtN}_a - \widetilde{\text{DtN}_a}\|$ small enough and (6.3) follow by a standard Neumann series argument. \square

To prove Theorem 13 we interpret the action of the sponge layer as an approximation of the DtN_a -operator.

Proof (Theorem 13) Let $\rho \geq \rho_0^{(\text{ext})}$. Define $\tilde{\mu} : H^1(\Omega_a) \times H^1(\Omega_a) \rightarrow \mathbb{C}$ as in (2.2) but DtN_a replaced by $\text{DtN}_{a,\rho}^{(\text{PML})}$. Since $\|\text{DtN}_a - \text{DtN}_{a,\rho}^{(\text{PML})}\| \leq C\rho e^{-\kappa\sigma\rho}$ (Lemma 12) the variational problem

$$\tilde{\mu}(u, v) = F(v), \text{ for all } v \in H^1(\Omega_a). \quad (6.4)$$

as a unique solution $u_\rho^{(\text{PML,int})} \in H^1(\Omega_a)$ for ρ large enough, and $\|u_\rho^{(\text{PML,int})} - u_\rho^{(\text{PML})}\|_{H^1(\Omega_a)} \leq C\rho e^{-\kappa\sigma\rho}$ by Lemma 14. Further, with $g = u_\rho^{(\text{PML,int})}|_{S_a^{d-1}} \in H^{1/2}(S_a^{d-1})$ the system (4.7) has a unique solution $u_\rho^{(\text{PML,ext})} \in H^1(D_{a,\rho})$. A straightfoward computation shows that

$$u_\rho^{(\text{PML})}(x) := \begin{cases} u_\rho^{(\text{PML,int})}(x), & x \in \Omega_a \\ u_\rho^{(\text{PML,ext})}(x), & x \in D_{a,\rho} \end{cases}$$

is a solution to (6.1). To prove uniqueness, we extend γ to Ω_a by $\gamma(r) = r$. Hence $\gamma' = 1$ in Ω_a . Accordingly we extend Δ_γ to Ω_a . A solution u to (6.1) satisfies $\Delta_\gamma u + k_\gamma^2 u = 0$ in Ω_ρ . It follows easily from Lemma 4 that the (extended) operator $\frac{\gamma'}{r} \Delta_\gamma$ is strongly elliptic. Due to the interior regularity theorem (see [10, Theorem 8.51]) for strongly elliptic equations we conclude that $\partial_r u|_{S_a^{d-1}}$ exists. Since the restriction of u to $D_{a,\infty}$ is the unique solution to (4.7) with $g = u|_{S_a^{d-1}} \in H^{1/2}(S_a^{d-1})$ we see that $\partial_r u|_{S_a^{d-1}} = \text{DtN}_{a,\rho}^{(\text{PML})} u|_{S_a^{d-1}}$. Therefore, the restriction of u to Ω_a is the unique solution $u_\rho^{(\text{PML,int})}$ to (6.4). In particular $u|_{S_a^{d-1}} = u_\rho^{(\text{PML,int})}$ and hence $u|_{D_{a,\rho}} = u_\rho^{(\text{PML,ext})}$. \square

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