

A QUASI-DUAL FUNCTION METHOD FOR EXTRACTING EDGE STRESS INTENSITY FUNCTIONS*

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Abstract. We present a method for the computation of the coefficients of singularities along the edges of a polyhedron for second-order elliptic boundary value problems. The class of problems considered includes problems of stress concentration along edges or crack fronts in general linear three-dimensional elasticity. Our method uses an incomplete construction of three-dimensional dual singular functions, based on explicitly known dual singular functions of two-dimensional problems tensorized by test functions along the edge and combined with complementary terms improving their orthogonality properties with respect to the edge singularities. Our method is aimed at the numerical computation of the stress intensity functions. It is suitable for a postprocessing procedure in the finite element approximation of the solution of the boundary value problem.

Key words. edge singularities, dual singularities, stress intensity factors

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1. Introduction.

1.1. The problem. The solutions of elliptic boundary problems, for example, those arising from linear elasticity, when posed and solved in nonsmooth domains like polygons and polyhedra, have nonsmooth parts. It is well known how to describe these singularities in terms of special *singular functions* depending on the geometry and the differential operators on one hand, and of unknown *coefficients* depending on the given right-hand sides (for example, volume forces and surface tractions or displacements) on the other hand.

Concerning the *singular functions*, they are extensively covered in the literature. In many cases, like corners in two dimensions or edges in three dimensions, they can be written analytically (see, for example, [18, 3, 29]) or semianalytically [12]. In other cases, like polyhedral corners, there exist well-known numerical methods for their computation (see, for example, [1, 35, 33, 36]).

Concerning the *coefficients*, there are two cases to distinguish: *corners* and *edges*.

1. In the case of a *corner* in two or three dimensions, i.e., the vertex of a cone, the space of singular functions up to a given regularity is finite-dimensional. Therefore only finitely many numbers have to be computed, and there exist several well-established methods to do this. Let us mention some of them:

In the “singular function method,” also known as the Fix method in the finite element literature, singular basis functions are added to the space of trial functions, so that their coefficients are computed immediately as a part of the numerical solution of the boundary value problem (see [4, 6, 8, 17, 28, 32]).

In the “dual singular function method,” one uses the fact that the coefficients depend linearly on the solution and therefore also on the right-hand side; see [21, 23]

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where this was first developed. There exist several different ways to express these linear functionals that extract the coefficients. One can use functionals acting on the solution of the boundary value problem, and these can then have a simple explicit form and can be localized. Or one can write them as functionals acting directly on the right-hand side. These are the dual singular functions, properly speaking, and they are solutions of a boundary value problem themselves (see [5, 15, 16, 7, 2, 34]).

2. In the case of an *edge* in three dimensions, the space of singular functions is infinite-dimensional. Theoretical formulas for the extraction of coefficients then involve an infinite number of dual singular functions in general; see [22, 26]. The coefficients can be understood as functions defined on the edge, and their computation now requires approximation of function spaces on the edge. There exist some papers describing versions of the singular function method in this case. In [13], the case of a half-space crack in three-dimensional elasticity is considered. An algorithm is proposed and analyzed consisting of boundary elements on the crack surface combined with singular elements that are parametrized by one-dimensional finite elements on the crack front. This method and the corresponding error analysis are described for smooth curved cracks in three dimensions in [31]. In [19], the simple case of a circular edge is treated with Fourier expansion, error estimates are given, and results of numerical computations are shown.

Every linear functional acting on the edge coefficient functions now gives rise to a dual singular function. Such linear functionals can be the point evaluation at each point of the edge or, more regularly, moments, i.e., scalar products with some polynomial basis functions. Computing a finite number of such point values or moments, one obtains an approximation of the coefficient function. Such a procedure has been studied in [20] for the simple case of the Laplace equation at a flat crack. In [30] the coefficients are given by convolution integrals which contain the dual singular functions, and examples for the Lamé system are provided.

With the exception of the computations in the case of the simple geometries and operators of [19] and [20], the formulas and theoretical algorithms for the extraction of *edge coefficients* mentioned above have not lead to numerical implementations or serious computational results. A first step towards an algorithm suitable for implementation in an engineering stress analysis code is described in [36], where point values of edge coefficients are computed in the case of the Laplace equation near a straight edge. Very special orthogonality conditions of the Laplace edge singular functions are used to construct extraction formulas that are essentially two-dimensional.

Whereas this idea cannot be extended directly to more general geometrical and physical situations like Lamé equations in a polyhedral domain, our paper is an extension of [36] to such situations in the practical sense of suitability for implementation in engineering codes.

1.2. Outline. In the present paper we construct an algorithm for the approximate computation of moments of the edge coefficient functions. The algorithm has a twofold purpose: It is sufficiently general to be applicable to real-life three-dimensional boundary value problems and their singularities near polyhedral edges, and it is simple enough to be implemented in the framework of professional finite element codes. In a forthcoming paper we will show practical applications in the computation of stress concentration coefficients in three-dimensional anisotropic elasticity.

Our paper is organized as follows:

After a more detailed description of the idea of our algorithm in this first section, we recall in section 2 the structure of edge singularities for second-order linear Dirichlet

boundary value problems in three dimensions. We describe how the leading term in each singular function is obtained from a two-dimensional problem in a sector and can be computed from the principal Mellin symbol of the partial differential operator. For a complete description of the singular function one has to construct higher order “shadow terms,” for which we also give formulas involving Mellin symbols of the operator.

In section 3, the structure of dual singular functions is described first in two dimensions and then for the case of the three-dimensional edge. The dual singular functions have an asymptotic expansion in terms that have tensor product form in cylindrical coordinates and are homogeneous with respect to the distance to the edge. This form allows us to prove a certain approximate duality between finite partial sums of these asymptotic expansions. These sums can be constructed explicitly from the Mellin symbols of the operator, and the duality holds approximately on cylindrical domains in the sense that the error is of the order of an arbitrarily high power of the radius of the cylinder.

In section 4, we construct the extraction algorithm for moments of the coefficients of the edge singularities. The algorithm requires the integration of the solution of the boundary value problem against a smooth function on a cylindrical surface of distance R to the edge, and it is exact modulo a given arbitrarily high power of R .

In section 5, we discuss generalizations to more general domains and boundary conditions, and the special case of a crack.

In section 6, we compare our algorithm with possible alternatives based on other formulas for the extraction of coefficients.

1.3. The main framework. Any three-dimensional elliptic boundary value problem posed on a polyhedron defines infinite-dimensional singularity spaces corresponding to each of the *edges*. Each singularity along an edge E is characterized

- by an *exponent* α , which is a complex number depending only on the geometry and the operator, and which determines the level of nonsmoothness of the singularity, and
- by a *coefficient* a_α , which is a function along the edge E .

Of great interest are the coefficients a_α when $\text{Re } \alpha$ is less than 1, corresponding to non- H^2 solutions. In many situations, $\text{Re } \alpha < 1$ when the opening at the edge is nonconvex. For example, α can be equal to $\frac{1}{2}$ in elasticity problems in the presence of cracks. Sometimes in such a situation the coefficients are called *stress intensity factors*. Herein we propose a method for the computation of these coefficients, which can be applied to any edge (including a crack front) of any polyhedron.

For the exposition of the method we use a model domain Ω where only one edge E is of interest (in particular, E will be the only possible nonconvex edge). Nevertheless this method applies, almost without alteration, to any polyhedron; see section 5.

As model domain, we take the tensor product $\Omega = G \times I$, where I is an interval, let us say $[-1, 1]$, and G is a plane bounded sector of opening $\omega \in (0, 2\pi]$ and radius 1 (the case of a crack, $\omega = 2\pi$, is included). See Figure 1. The variables are (x, y) in G and z in I , and we denote the coordinates (x, y, z) by \mathbf{x} . Let (r, θ) be the polar coordinates centered at the vertex of G so that $G = \{(x, y) \in \mathbb{R}^2 \mid r \in (0, 1), \theta \in (0, \omega)\}$. The domain Ω has an *edge* E which is the set $\{(x, y, z) \in \mathbb{R}^3 \mid r = 0, z \in I\}$.

The operator L is a homogeneous second-order partial differential $N \times N$ system with constant real coefficients, which means that

$$L = \sum_{j=1}^3 \sum_{i=1}^3 L_{ij} \partial_i \partial_j \quad \text{with} \quad \partial_1 = \frac{\partial}{\partial x}, \quad \partial_2 = \frac{\partial}{\partial y}, \quad \partial_3 = \frac{\partial}{\partial z},$$

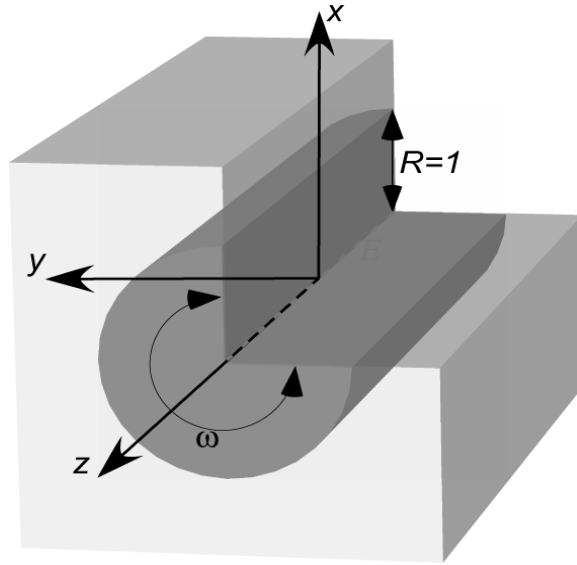


FIG. 1. The domain of interest Ω .

with coefficient matrices L_{ij} in $\mathbb{R}^{N \times N}$. We moreover assume that the matrices L_{ij} are symmetric. Therefore L is formally self-adjoint.

We assume moreover that L is associated with an elliptic bilinear form B , i.e., that for any u and v in $H^2(\Omega)^N$ and any subdomain $\Omega' \subset \Omega$ there holds

$$\begin{aligned}
 (1.1) \quad \int_{\Omega'} Lu \cdot v \, d\mathbf{x} &= B(u, v) + \int_{\Gamma'} T_{\Gamma'} u \cdot v \, d\sigma \\
 &= \int_{\Omega'} u \cdot Lv \, d\mathbf{x} + \int_{\Gamma'} (T_{\Gamma'} u \cdot v - u \cdot T_{\Gamma'} v) \, d\sigma,
 \end{aligned}$$

where $T_{\Gamma'}$ is the Neumann trace operator associated with L via B on the boundary Γ' of Ω' . Our aim is the determination of the edge structure of any solution u of the problem

$$(1.2) \quad u \in H_0^1(\Omega) \quad \forall v \in H_0^1(\Omega) \quad B(u, v) = \int_{\Omega} f \cdot v \, d\mathbf{x},$$

where f is a smooth vector function in $C^\infty(\bar{\Omega})^N$. Away from the end points of the edge, the solution u can be expanded in edge singularities $S[\alpha; a_\alpha]$ associated with the exponents α and the coefficients a_α . These singularities $S[\alpha; a_\alpha]$ are the sums of terms in tensor product form $\partial_z^j a_\alpha(z) \Phi_j[\alpha](x, y)$, where only the generating coefficients a_α depend on the right-hand side f of problem (1.2).

1.4. The extraction method. In this paper, we construct for each exponent α a set of *quasi-dual* singular functions $K^m[\alpha; b]$, where m is a natural integer, which is the *order* of the quasi-dual function, and b a test coefficient. We then extract not the pointwise values of a_α , but its scalar product versus b on E with the help of the following *antisymmetric* internal boundary integrals $J[R]$ over the surface

$$\Gamma_R := \{ \mathbf{x} \in \mathbb{R}^3 \mid r = R, \theta \in (0, \omega), z \in I \},$$

depending on the radius R :

$$(1.3) \quad J[R](u, v) := \int_{\Gamma_R} (T_{\Gamma_R} u \cdot \bar{v} - u \cdot T_{\Gamma_R} \bar{v}) \, d\sigma.$$

Roughly, and with certain limitations (see Theorem 4.3 and its extensions in section 5), we find that for the lowest values of $\operatorname{Re} \alpha$, there holds

$$(1.4) \quad J[R](u, K^m[\alpha; b]) = \int_I a_\alpha(z) \bar{b}(z) \, dz + \mathcal{O}(R^{m+1}) \quad \text{as } R \rightarrow 0,$$

which allows a precise determination of $\int_I a_\alpha \bar{b}$ by extrapolation in R and a reconstruction of a_α by the choice of a suitable set of test coefficients b .

One of the fundamental tools for the proof of (1.4) consists of algebraic relations based on integration by parts in the domains $\Omega_{\varepsilon,R}$, where for any ε and R with $0 < \varepsilon < R$ we denote by $G_{\varepsilon,R}$ the annulus

$$G_{\varepsilon,R} := \{(x, y) \in \mathbb{R}^2 \mid r \in (\varepsilon, R), \theta \in (0, \omega)\}$$

and by $\Omega_{\varepsilon,R}$ the tensor domain $G_{\varepsilon,R} \times I$. We note that

$$\partial\Omega_{\varepsilon,R} = \Gamma_\varepsilon \cup \Gamma_R \cup (G_{\varepsilon,R} \times \partial I).$$

Finally we also denote by G_∞ the infinite sector of opening ω and by Ω_∞ the infinite wedge $G_\infty \times I$.

2. Edge singularities. Edge singularities are investigated in several works. Let us quote Maz'ya and Plamenevskii [24], Maz'ya and Rossmann [27], Dauge [14], and Costabel and Dauge [9]. Here, as a model problem, we concentrate on the simplest case of a homogeneous operator with constant coefficients.

The structure and the expansion of edge singularities rely on the splitting of the operator L into three parts,

$$L = M_0(\partial_x, \partial_y) + M_1(\partial_x, \partial_y) \partial_z + M_2 \partial_z^2,$$

where M_0 is an $N \times N$ matrix of second-order partial differential operators in (x, y) , M_1 is an $N \times N$ matrix of first-order partial differential operators in (x, y) , and M_2 is a scalar $N \times N$ matrix.

We can check that for any smooth function $a(z)$ in I and any sequence $(\Phi_j)_{j \geq 0}$ of functions of (x, y) satisfying the relations

$$(2.1) \quad \begin{cases} M_0 \Phi_0 = 0, \\ M_0 \Phi_1 + M_1 \Phi_0 = 0, \\ M_0 \Phi_j + M_1 \Phi_{j-1} + M_2 \Phi_{j-2} = 0, \end{cases} \quad j \geq 2, \quad \text{in } G_\infty,$$

the series

$$u \sim \sum_{j \geq 0} \partial_z^j a(z) \Phi_j(x, y)$$

formally satisfies the equation $Lu \sim 0$ in Ω_∞ . If, moreover, all derivatives of a are zero in ± 1 and if the Φ_j satisfy the Dirichlet conditions on ∂G_∞ , then $u \sim 0$ on $\partial\Omega_\infty$. In order to provide a more precise meaning, we need a description of solutions of the system of equations (2.1).

2.1. Two-dimensional leading singularities. The first terms Φ_0 are the solutions of the Dirichlet problem in the infinite sector:

$$(2.2) \quad \begin{cases} M_0\Phi_0 = 0 & \text{in } G_\infty, \\ \Phi_0 = 0 & \text{on } \partial G_\infty. \end{cases}$$

From the general theory we know that the solutions of problem (2.2) are generated by functions having the particular form in polar coordinates (r, θ)

$$(2.3) \quad \Phi_0 = r^\alpha \varphi_0(\theta), \quad \alpha \in \mathbb{C}.$$

Since it is homogeneous of degree 2, the system M_0 can be written in polar coordinates in the form

$$M_0(\partial_x, \partial_y) = r^{-2} \mathcal{M}_0(\theta; r\partial_r, \partial_\theta).$$

With the ansatz (2.3), the system (2.2) becomes

$$(2.4) \quad \begin{cases} \mathcal{M}_0(\theta; \alpha, \partial_\theta)\varphi_0 = 0 & \text{in } (0, \omega), \\ \varphi_0 = 0 & \text{on } 0 \text{ and } \omega. \end{cases}$$

The operator $\varphi \mapsto \mathcal{M}_0(\theta; \alpha, \partial_\theta)\varphi$ acting from $H_0^1(0, \omega)$ into $H^{-1}(0, \omega)$ is the *Mellin symbol* of M_0 , and we denote it by $\mathfrak{M}_0(\alpha)$.

The system (2.4) has nonzero solutions, i.e., $\mathfrak{M}_0(\alpha)$ is not invertible, only for a discrete subset $\mathfrak{A} = \mathfrak{A}(M_0)$ of \mathbb{C} . We call the numbers $\alpha \in \mathfrak{A}$ the *edge exponents*.

The ellipticity of L implies the ellipticity of M_0 , and as a consequence, any strip $\text{Re } \alpha \in (\xi_1, \xi_2)$ contains at most a finite number of elements of \mathfrak{A} . As the coefficients of M_0 are real, if α belongs to \mathfrak{A} , then $\bar{\alpha}$ also belongs to \mathfrak{A} . Moreover we have the general property that

$$\mathfrak{M}_0(\alpha)^* = \mathfrak{M}_0^*(-\bar{\alpha}),$$

where $\mathfrak{M}_0(\alpha)^*$ is the adjoint of $\mathfrak{M}_0(\alpha)$ and \mathfrak{M}_0^* denotes the Mellin symbol of the adjoint M_0^* of M_0 . Now M_0 is formally self-adjoint: $M_0^* = M_0$, and there holds

$$\mathfrak{M}_0(\alpha)^* = \mathfrak{M}_0(-\bar{\alpha}).$$

By the Fredholm alternative, this implies that if α belongs to \mathfrak{A} , then $-\bar{\alpha}$ also belongs to \mathfrak{A} .

The operator valued function $\alpha \mapsto \mathfrak{M}_0(\alpha)^{-1}$ is meromorphic on \mathbb{C} . If

$$(\mathfrak{H}_1) \quad \forall \alpha \in \mathfrak{A}, \quad \alpha \text{ is a pole of degree 1 of } \mathfrak{M}_0^{-1},$$

then any solution of (2.2) is a linear combination of solutions of type (2.3) with $\alpha \in \mathfrak{A}$ and φ_0 a nonzero solution of (2.4). For simplicity we assume hypothesis (\mathfrak{H}_1) and will explain in what follows the implications if it does not hold.

2.2. Further two-dimensional generators for singularities. The second equation of system (2.1) with Dirichlet conditions reduces to finding Φ_1 such that

$$(2.5) \quad \begin{cases} M_0\Phi_1 = -M_1\Phi_0 & \text{in } G_\infty, \\ \Phi_1 = 0 & \text{on } \partial G_\infty, \end{cases}$$

where $\Phi_0 = r^\alpha \varphi_0(\theta)$ as determined in the previous subsection. Since it is homogeneous of degree 1, the system M_1 can be written in polar coordinates in the form

$$M_1(\partial_x, \partial_y) = r^{-1} \mathcal{M}_1(\theta; r\partial_r, \partial_\theta).$$

Therefore, $M_1 \Phi_0 = r^{\alpha-1} \mathcal{M}_1(\theta; \alpha, \partial_\theta) \varphi_0$ and an ansatz like (2.3) for the solution of problem (2.5) is

$$(2.6) \quad \Phi_1 = r^{\alpha+1} \varphi_1(\theta),$$

with φ_1 solution of the Dirichlet problem

$$(2.7) \quad \begin{cases} \mathcal{M}_0(\theta; \alpha + 1, \partial_\theta) \varphi_1 = -\mathcal{M}_1(\theta; \alpha, \partial_\theta) \varphi_0 & \text{in } (0, \omega), \\ \varphi_1 = 0 & \text{on } 0 \text{ and } \omega; \end{cases}$$

in other words, φ_1 solves $\mathfrak{M}_0(\alpha + 1) \varphi_1 = -\mathcal{M}_1(\alpha) \varphi_0$. Therefore, if $\alpha + 1$ does not belong to \mathfrak{A} , the previous problem has a unique solution. This is why we assume hypothesis (\mathfrak{H}_2) :

$$(\mathfrak{H}_2) \quad \forall \alpha \in \mathfrak{A}, \quad \forall j \in \mathbb{N}, j \geq 1, \quad \alpha + j \notin \mathfrak{A}.$$

If (\mathfrak{H}_2) holds, then for each solution $\Phi_0 = r^\alpha \varphi_0$ of problem (2.4), we obtain by induction a unique sequence $(\Phi_j)_{j \geq 0}$ solution of (2.1) with Dirichlet conditions in the form

$$\Phi_j = r^{\alpha+j} \varphi_j(\theta),$$

where φ_j solves

$$(2.8) \quad \mathfrak{M}_0(\alpha + j) \varphi_j = -\mathcal{M}_1(\alpha + j - 1) \varphi_{j-1} - M_2 \varphi_{j-2}.$$

We recall that M_2 , being a scalar matrix, has the same expression in Cartesian coordinates as in polar coordinates (viz. $M_2 = \mathcal{M}_2$).

2.3. Three-dimensional singularities. Assuming hypotheses (\mathfrak{H}_1) and (\mathfrak{H}_2) , for any $\alpha \in \mathfrak{A}$ with $\text{Re } \alpha > 0$, let p_α denote the dimension of the kernel of $\mathfrak{M}_0(\alpha)$ and let $\Phi_0[\alpha, p]$, for $p = 1, \dots, p_\alpha$, be a basis of $\ker \mathfrak{M}_0(\alpha)$. Moreover, for any $j \geq 1$, let $\Phi_j[\alpha, p]$ be the solution of (2.7) or (2.8) (also called “*shadow singularities*”) generated by $\Phi_0[\alpha, p]$.

For any integer $n \geq 0$ we call “*singularity at the order n*” any expression of the form

$$(2.9) \quad S^n[\alpha, p; a] := \sum_{j=0}^n \partial_z^j a(z) \Phi_j[\alpha, p](x, y),$$

where a belongs to $\mathcal{C}^{n+2}(\bar{I})$.

By construction, there holds

$$(2.10) \quad LS^n[\alpha, p; a] = \partial_z^{n+1} a (M_1 \Phi_n + M_2 \Phi_{n-1}) + \partial_z^{n+2} a M_2 \Phi_n,$$

whence we have the following lemma.

LEMMA 2.1. *For any $\alpha \in \mathfrak{A}$, $\text{Re } \alpha > 0$, and $a \in \mathcal{C}^{n+2}(\bar{I})$ we have*

$$(2.11) \quad LS^n[\alpha, p; a] = \mathcal{O}(r^{\text{Re } \alpha + n - 1});$$

i.e., $r^{-\text{Re } \alpha - n + 1} LS^n[\alpha, p; a]$ is bounded in $\bar{\Omega}$. Moreover $S^n[\alpha, p; a] = 0$ on $\partial G_\infty \times I$.

3. Dual singular functions. We first recall and reformulate well-known facts about the dual singular functions for two-dimensional problems (cf. Maz'ya and Plamenevskii [21, 23, 25], Babuška and Miller [2], Dauge et al. [15, 16]) and then extend these notions in the framework of our edge problem, so that we obtain what we call “*quasi-dual singular functions*” (compare with the extraction functions in [1] by Andersson, Falk, and Babuška) as opposed to exact dual singular functions; cf. Maz'ya and Plamenevskii [22], Maz'ya and Rossmann [26] (pointwise duality), and Lenczner [20] (Sobolev duality).

3.1. Two-dimensional dual singular functions. The two-dimensional operator is the homogeneous second-order operator M_0 with real coefficients. We develop its symbol $\mathcal{M}_0(\alpha)$ in powers of α (of degree 2):

$$(3.1) \quad \mathcal{M}_0(\theta; \alpha, \partial_\theta) = \mathcal{N}_0(\theta; \partial_\theta) + \alpha \mathcal{N}_1(\theta; \partial_\theta) + \alpha^2 \mathcal{N}_2(\theta).$$

Since M_0 is self-adjoint, we can deduce that

$$(3.2) \quad \mathcal{N}_0 \text{ and } \mathcal{N}_2 \text{ are self-adjoint and } \mathcal{N}_1 \text{ is anti-self-adjoint.}$$

LEMMA 3.1. *Let α, β be in \mathfrak{A} and let φ, ψ be in the kernels of $\mathfrak{M}_0(\alpha), \mathfrak{M}_0(\beta)$, respectively. Then there holds the identity*

$$(3.3) \quad (\alpha + \bar{\beta}) \int_0^\omega (\mathcal{N}_1 + (\alpha - \bar{\beta})\mathcal{N}_2)\varphi \cdot \bar{\psi} \, d\theta = 0.$$

Proof. We start with the duality relation:

$$0 = \int_0^\omega \varphi \cdot \overline{\mathfrak{M}_0(\beta)\psi} = \int_0^\omega \mathfrak{M}_0(\beta)^* \varphi \cdot \bar{\psi} = \int_0^\omega \mathfrak{M}_0(-\bar{\beta})\varphi \cdot \bar{\psi}.$$

Then we use the identity

$$\mathfrak{M}_0(-\bar{\beta}) = \mathfrak{M}_0(\alpha) - (\bar{\beta} + \alpha)\mathcal{N}_1 + (\bar{\beta}^2 - \alpha^2)\mathcal{N}_2.$$

From $\mathfrak{M}_0(\alpha)\varphi = 0$, we obtain

$$\begin{aligned} 0 &= \int_0^\omega \mathfrak{M}_0(-\bar{\beta})\varphi \cdot \bar{\psi} = \int_0^\omega (-(\bar{\beta} + \alpha)\mathcal{N}_1 + (\bar{\beta}^2 - \alpha^2)\mathcal{N}_2)\varphi \cdot \bar{\psi} \\ &= -(\alpha + \bar{\beta}) \int_0^\omega (\mathcal{N}_1 + (\alpha - \bar{\beta})\mathcal{N}_2)\varphi \cdot \bar{\psi}. \quad \square \end{aligned}$$

LEMMA 3.2. *Let α, β, φ , and ψ be as in Lemma 3.1.*

(i) *If $-\bar{\beta} \neq \alpha$, then*

$$(3.4) \quad \int_0^\omega (\mathcal{N}_1 + (\alpha - \bar{\beta})\mathcal{N}_2)\varphi \cdot \bar{\psi} = 0.$$

(ii) *If $-\bar{\beta} = \alpha$, then the left-hand side of (3.4) becomes*

$$(3.5) \quad \int_0^\omega (\mathcal{N}_1 + 2\alpha\mathcal{N}_2)\varphi \cdot \bar{\psi} = \int_0^\omega \left(\frac{d}{d\alpha} \mathfrak{M}_0(\alpha) \right) \varphi \cdot \bar{\psi},$$

and, if we moreover assume hypothesis (\mathfrak{H}_1) , then for any basis $(\varphi[\alpha, p])_p$ of $\ker \mathfrak{M}_0(\alpha)$ there exists a unique dual basis $(\bar{\psi}[\alpha, p])_p$ of $\ker \mathfrak{M}_0(-\bar{\alpha})$ such that

$$(3.6) \quad \int_0^\omega (\mathcal{N}_1 + 2\alpha\mathcal{N}_2)\varphi[\alpha, p] \cdot \bar{\psi}[\alpha, q] = \delta_{p,q}.$$

Proof. (i) is a straightforward consequence of Lemma 3.1.

(ii) Identity (3.5) is clear. Concerning (3.6), we first note that since $\mathfrak{M}_0(\alpha)^* = \mathfrak{M}_0(-\bar{\alpha})$, the dimension of the kernel of $\mathfrak{M}_0(\alpha)$ is equal to the codimension of the closure of the range of $\mathfrak{M}_0(-\bar{\alpha})$. On the other hand, as for any $\alpha' \in \mathbb{C} \setminus \mathfrak{A}$, $\mathfrak{M}_0(\alpha')$ is invertible, and since $\mathfrak{M}_0(\alpha) - \mathfrak{M}_0(\alpha')$ is a compact operator, $\mathfrak{M}_0(\alpha)$ is a Fredholm operator of index 0. As a consequence,

$$\dim \ker \mathfrak{M}_0(\alpha) = \dim \ker \mathfrak{M}_0(-\bar{\alpha}).$$

In order to obtain (3.6) it suffices now to prove that if $\varphi \in \ker \mathfrak{M}_0(\alpha)$ satisfies

$$\forall \psi \in \ker \mathfrak{M}_0(-\bar{\alpha}), \quad \int_0^\omega (\mathcal{N}_1 + 2\alpha\mathcal{N}_2)\varphi \cdot \bar{\psi} = 0,$$

then $\varphi = 0$. If this does not hold, thanks to (3.5) there exists $\varphi \in \ker \mathfrak{M}_0(\alpha)$ such that

$$\forall \psi \in \ker \mathfrak{M}_0(-\bar{\alpha}), \quad \int_0^\omega \left(\frac{d}{d\alpha} \mathfrak{M}_0(\alpha) \right) \varphi \cdot \bar{\psi} = 0.$$

By the Fredholm alternative, there exists φ' such that

$$\mathfrak{M}_0(\alpha)\varphi' + \frac{d}{d\alpha} \mathfrak{M}_0(\alpha)\varphi = 0.$$

As a consequence the function

$$\alpha' \longmapsto (\alpha' - \alpha)^{-2} \mathfrak{M}_0(\alpha')(\varphi + (\alpha' - \alpha)\varphi')$$

has an analytic extension in α . This contradicts hypothesis (\mathfrak{H}_1) according to which \mathfrak{M}_0^{-1} has a pole of order 1 in α . \square

We end this subsection with a relation between the expression in the left-hand sides of (3.4) and (3.6) and a trace obtained by integration by parts.

Considering the Green formula (1.1) in the domain $\Omega_{\varepsilon,R}$ for functions u and v , which are zero on the two faces $\theta = 0$ and $\theta = \omega$ of Ω , we have contributions on the parts Γ_R and Γ_ε of the boundary of $\Omega_{\varepsilon,R}$, where $r = R$ and $r = \varepsilon$, respectively. We denote by $T(r)$ the Neumann trace operator on Γ_r . It has the form

$$(3.7) \quad T(r) = T(r, \theta; \partial_r, \partial_\theta, \partial_z) = r^{-1}T_0(\theta; r\partial_r, \partial_\theta) + T_1(\theta) \partial_z.$$

We also have contributions of the lateral sides $G_{\varepsilon,R} \times \partial I$. Denoting by $T_{\partial I}$ the Neumann trace on these sides, we have the Green formula

$$(3.8) \quad \begin{aligned} \int_{\Omega_{\varepsilon,R}} Lu \cdot v - u \cdot Lv \, d\mathbf{x} &= \int_I \int_0^\omega T(R)u \cdot v - u \cdot T(R)v \, R \, d\theta \, dz \\ &\quad - \int_I \int_0^\omega T(\varepsilon)u \cdot v - u \cdot T(\varepsilon)v \, \varepsilon \, d\theta \, dz \\ &\quad + \int_{G_{\varepsilon,R} \times \partial I} T_{\partial I} u \cdot v - u \cdot T_{\partial I} v \, d\sigma. \end{aligned}$$

Applying the above identity to functions u and v independent of z (and zero on the two sides $\theta = 0$ and $\theta = \omega$), we note that the contributions on the two sides $G_{\varepsilon,R} \times \{\pm 1\}$ cancel out because the two Neumann operators $T_{\pm 1}$ which compose $T_{\partial I}$ are opposite to each other. Thus we obtain

$$(3.9) \quad \int_{G_{\varepsilon,R}} M_0 u \cdot v - u \cdot M_0 v \, dx \, dy = \int_0^\omega T_0(R)u \cdot v - u \cdot T_0(R)v \, d\theta - \int_0^\omega T_0(\varepsilon)u \cdot v - u \cdot T_0(\varepsilon)v \, d\theta,$$

where $T_0(R)$ denotes $T_0(\theta; R\partial_r, \partial_\theta)$.

LEMMA 3.3. *Let α and β be complex numbers and let φ and ψ belong to $H_0^1(0, \omega)^N$. Set $\Phi := r^\alpha \varphi(\theta)$ and $\Psi := r^{-\beta} \psi(\theta)$. For any $R > 0$ there holds*

$$(3.10) \quad \int_0^\omega T_0(R)\Phi \cdot \bar{\Psi} - \Phi \cdot T_0(R)\bar{\Psi} \, d\theta = R^{\alpha-\beta} \int_0^\omega (\mathcal{N}_1 + (\alpha + \beta)\mathcal{N}_2)\varphi \cdot \bar{\psi} \, d\theta.$$

Proof. Formula (3.9) and the splitting (3.1) of $\mathcal{M}_0 = r^2 M_0$ yield for any $\varepsilon < R$

$$\begin{aligned} \int_{G_{\varepsilon,R}} \left((\mathcal{N}_0 + r\partial_r \mathcal{N}_1 + (r\partial_r)^2 \mathcal{N}_2)\Phi \cdot \bar{\Psi} - \Phi \cdot (\mathcal{N}_0 + r\partial_r \mathcal{N}_1 + (r\partial_r)^2 \mathcal{N}_2)\bar{\Psi} \right) \frac{1}{r} \, dr \, d\theta \\ = \int_0^\omega T_0(R)\Phi \cdot \bar{\Psi} - \Phi \cdot T_0(R)\bar{\Psi} \, d\theta \\ - \int_0^\omega T_0(\varepsilon)\Phi \cdot \bar{\Psi} - \Phi \cdot T_0(\varepsilon)\bar{\Psi} \, d\theta. \end{aligned}$$

Since \mathcal{N}_0 is self-adjoint, integration by parts gives

$$\begin{aligned} \int_\varepsilon^R \left((\mathcal{N}_0 + r\partial_r \mathcal{N}_1 + (r\partial_r)^2 \mathcal{N}_2)\Phi \cdot \bar{\Psi} - \Phi \cdot (\mathcal{N}_0 + r\partial_r \mathcal{N}_1 + (r\partial_r)^2 \mathcal{N}_2)\bar{\Psi} \right) \frac{1}{r} \, dr \\ = [\mathcal{N}_1 \Phi \cdot \bar{\Psi} + (r\partial_r)\mathcal{N}_2 \Phi \cdot \bar{\Psi} - \Phi \cdot (r\partial_r)\mathcal{N}_2 \bar{\Psi}]_\varepsilon^R. \end{aligned}$$

We have

$$\mathcal{N}_1 \Phi \cdot \bar{\Psi} + (r\partial_r)\mathcal{N}_2 \Phi \cdot \bar{\Psi} - \mathcal{N}_2 \Phi \cdot (r\partial_r)\bar{\Psi} = r^{\alpha-\beta} (\mathcal{N}_1 \varphi \cdot \bar{\psi} + \alpha \mathcal{N}_2 \varphi \cdot \bar{\psi} + \varphi \cdot \beta \mathcal{N}_2 \bar{\psi}),$$

and as \mathcal{N}_2 is self-adjoint (cf. (3.2)), we finally obtain

$$\begin{aligned} (\mathcal{N}_1 \varphi \cdot \bar{\psi} + (\alpha + \beta)\mathcal{N}_2 \varphi \cdot \bar{\psi})(R^{\alpha-\beta} - \varepsilon^{\alpha-\beta}) &= \int_0^\omega T_0(R)\Phi \cdot \bar{\Psi} - \Phi \cdot T_0(R)\bar{\Psi} \, d\theta \\ &- \int_0^\omega T_0(\varepsilon)\Phi \cdot \bar{\Psi} - \Phi \cdot T_0(\varepsilon)\bar{\Psi} \, d\theta. \end{aligned}$$

Now the right-hand side of the above equality also has the form $c(\alpha, \beta)(R^{\alpha-\beta} - \varepsilon^{\alpha-\beta})$, and we deduce (3.10) for any $\alpha \neq \beta$. Since, for fixed β, φ, ψ , and R , both members of (3.10) depend continuously on α , we deduce (3.10) for $\alpha = \beta$ by continuity. \square

3.2. Three-dimensional dual singular functions. We assume hypotheses (\mathfrak{H}_1) and (\mathfrak{H}_2) , and for any $\alpha \in \mathfrak{A}$, $\text{Re } \alpha > 0$, we choose a basis $\varphi[\alpha, p]$, $p = 1, \dots, p_\alpha$, of $\ker \mathfrak{M}_0(\alpha)$. Then we denote by $\psi[\alpha, p]$, $p = 1, \dots, p_\alpha$, the corresponding dual basis according to Lemma 3.2. We recall that we have denoted $r^\alpha \varphi[\alpha, p]$ by $\Phi_0[\alpha, p]$ and that associated singularities at the order n are defined in (2.9).

Following the same lines, we set

$$\Psi_0[\alpha, p] := r^{-\bar{\alpha}}\psi[\alpha, p],$$

and for any integer $n \geq 0$, we define the “quasi-dual singular function at the order n ” by

$$(3.11) \quad K^n[\alpha, p; b] := \sum_{j=0}^n \partial_z^j b(z) \Psi_j[\alpha, p](x, y),$$

where b belongs to $\mathcal{C}^{n+2}(\bar{I})$ and the sequence $(\Psi_j)_{j \geq 0}$ is defined by induction as solution of (2.1) in the form

$$\Psi_j = r^{-\bar{\alpha}+j}\psi_j(\theta),$$

where ψ_j solves

$$(3.12) \quad \mathfrak{M}_0(-\bar{\alpha} + j)\psi_j = -\mathcal{M}_1(-\bar{\alpha} + j - 1)\psi_{j-1} - M_2\psi_{j-2}.$$

Of course, $K^n[\alpha, p; b]$ is but $S^n[-\bar{\alpha}, p; b]$ (generated by Ψ_0). Therefore by (2.11) there holds, for any $\alpha \in \mathfrak{A}$, $\text{Re } \alpha > 0$, and $b \in \mathcal{C}^{n+2}(\bar{I})$,

$$(3.13) \quad LK^n[\alpha, p; b] = \mathcal{O}(r^{-\text{Re } \alpha + n - 1}).$$

In the next proposition we state that the singularities $S^n[\alpha, p; a]$ and the quasi-dual singular functions $K^n[\beta, q; b]$ are in duality with each other (modulo a remainder) if linked by the following antisymmetric sesquilinear form:

$$(3.14) \quad J[R](u, v) := \int_{\Gamma_R} (Tu \cdot \bar{v} - u \cdot T\bar{v}) \, d\sigma = \int_I \int_0^\omega (Tu \cdot \bar{v} - u \cdot T\bar{v})|_{r=R} R \, d\theta \, dz,$$

where $T = T(R)$ is the radial Neumann trace operator (3.7).

PROPOSITION 3.4. *Let $\alpha, \beta \in \mathfrak{A}$ with $\text{Re } \alpha, \text{Re } \beta > 0$. We assume that hypotheses (\mathfrak{H}_1) and (\mathfrak{H}_2) hold. For an integer $n \geq 0$, let the coefficients a and b be in $\mathcal{C}^{n+2}(\bar{I})$. We assume moreover that $\partial_z^j b = 0$ for $j = 0, \dots, n - 1$ on ∂I . Then for any $R > 0$ there holds*

$$(3.15) \quad J[R](S^n[\alpha, p; a], K^n[\beta, q; b]) = \delta_{\alpha, \beta} \delta_{p, q} \int_I a(z) \bar{b}(z) \, dz + \mathcal{O}(R^{\text{Re } \alpha - \text{Re } \beta + n + 1}).$$

Proof. We use the Green formula (3.8) on $G_{\varepsilon, R}$ for

$$u = S^n[\alpha, p; a] \quad \text{and} \quad v = \overline{K^n[\alpha, q; b]}.$$

Since $u = \mathcal{O}(r^{\text{Re } \alpha})$ and $v = \mathcal{O}(r^{-\text{Re } \beta})$, (2.11) and (3.13) imply

$$\int_{\Omega_{\varepsilon, R}} Lu \cdot v - u \cdot Lv \, d\mathbf{x} = \mathcal{O}\left(\int_\varepsilon^R r^{\text{Re } \alpha - \text{Re } \beta + n - 1} r \, dr\right).$$

With formula (2.10), we even obtain the more precise expression

$$\int_{\Omega_{\varepsilon, R}} Lu \cdot v - u \cdot Lv \, d\mathbf{x} = \sum_{k=n-1}^{2n} \gamma_k \int_\varepsilon^R r^{\alpha - \beta + k} r \, dr,$$

with coefficients γ_k independent of R and ε . As a consequence of hypothesis (\mathfrak{H}_2) we know that $\alpha - \beta + k$ is different from -1 for $k = n, \dots, 2n + 1$. Thus

$$\int_{\Omega_{\varepsilon,R}} Lu \cdot v - u \cdot Lv \, d\mathbf{x} = \sum_{k=n+1}^{2n+2} \lambda_k (R^{\alpha-\beta+k} - \varepsilon^{\alpha-\beta+k}),$$

with coefficients λ_k independent of R and ε . For the boundary integral $J[r](u, v)$ (3.14), we omit the mention of (u, v) . Thus the Green formula (3.8) gives

$$J[R] - J[\varepsilon] + \int_{G_{\varepsilon,R} \times \partial I} T_{\partial I} u \cdot v - u \cdot T_{\partial I} v \, r \, dr \, d\theta = \sum_{k=n+1}^{2n+2} \lambda_k (R^{\alpha-\beta+k} - \varepsilon^{\alpha-\beta+k}).$$

As $T_{\partial I}$ is of the form $r^{-1}T_{\partial I,0}(\theta; r\partial_r, \partial_\theta) + T_{\partial I,1}(\theta) \partial_z$ (cf. (3.7)), and as the ends ∂I are zeros of order n of b , we are left with

$$T_{\partial I} u \cdot v - u \cdot T_{\partial I} v = T_{\partial I} u \cdot \partial_z^n b \Psi_n - u \cdot \partial_z^n b (r^{-1}T_{\partial I,0} \Psi_n + T_{\partial I,1} \Psi_{n-1}) - u \cdot \partial_z^{n+1} b T_{\partial I,1} \Psi_n.$$

Integrating on $G_{\varepsilon,R} \times \partial I$ and using the structure of Ψ_j , we obtain as before

$$T_{\partial I} u \cdot v - u \cdot T_{\partial I} v = \sum_{k=n+1}^{2n+2} \lambda'_k (R^{\alpha-\beta+k} - \varepsilon^{\alpha-\beta+k}).$$

From the last three equalities we obtain

$$(3.16) \quad J[R] - J[\varepsilon] = \sum_{k=n+1}^{2n+2} \lambda''_k (R^{\alpha-\beta+k} - \varepsilon^{\alpha-\beta+k}).$$

It remains to expand $J[r]$ in homogeneous parts: we have

$$(3.17) \quad J[r] = \sum_{k=0}^{2n+1} J_k r^{\alpha-\beta+k}$$

with (cf. (3.7))

$$(3.18) \quad \begin{aligned} J_k &= \sum_{j+\ell=k} \int_I \int_0^\omega \partial_z^j a \partial_z^\ell \bar{b} \left(T_0(\theta; \alpha + j, \partial_\theta) \varphi_j \cdot \bar{\psi}_\ell - \varphi_j \cdot T_0(\theta; -\beta + \ell, \partial_\theta) \bar{\psi}_\ell \right) d\theta dz \\ &+ \sum_{j+\ell=k-1} \int_I \int_0^\omega \left(\partial_z^{j+1} a \partial_z^\ell \bar{b} T_1(\theta) \varphi_j \cdot \bar{\psi}_\ell - \partial_z^j a \partial_z^{\ell+1} \bar{b} \varphi_j \cdot T_1(\theta) \bar{\psi}_\ell \right) d\theta dz. \end{aligned}$$

Combining (3.16) with (3.17) we obtain

$$\sum_{k=0}^{2n+1} J_k (R^{\alpha-\beta+k} - \varepsilon^{\alpha-\beta+k}) = \sum_{k=n+1}^{2n+2} \lambda''_k (R^{\alpha-\beta+k} - \varepsilon^{\alpha-\beta+k}).$$

By identification of terms, we immediately deduce that

$$\forall k \leq n, \quad J_k (R^{\alpha-\beta+k} - \varepsilon^{\alpha-\beta+k}) = 0.$$

Therefore

$$\forall k \leq n \text{ such that } \alpha - \beta + k \neq 0, \quad J_k = 0.$$

By hypothesis (\mathfrak{H}_2) , the number $\alpha - \beta + k$ can be 0 only if $k = 0$. Therefore

$$\forall k, 1 \leq k \leq n, \quad J_k = 0 \quad \text{and} \quad \forall \alpha, \beta \in \mathfrak{A}, \quad \alpha \neq \beta, \quad J_0 = 0.$$

In order to obtain (3.15), it remains to study J_0 when $\alpha = \beta$. Formula (3.18) yields, for J_0 ,

$$J_0 = \int_I \int_0^\omega a \bar{b} \left(T_0(\theta; \alpha, \partial_\theta) \varphi_0[\alpha, p] \cdot \bar{\psi}_0[\alpha, q] - \varphi_j[\alpha, p] \cdot T_0(\theta; -\beta, \partial_\theta) \bar{\psi}_0[\alpha, q] \right) d\theta dz.$$

Applying Lemma 3.3 for $\alpha = \beta$ we have

$$J_0 = \left(\int_I a \bar{b} dz \right) \left(\int_0^\omega (\mathcal{N}_1 + 2\alpha \mathcal{N}_2) \varphi[\alpha, p] \cdot \bar{\psi}[\alpha, q] d\theta \right),$$

and with the orthogonality relation (3.6) we deduce that

$$J_0 = \delta_{p,q} \int_I a \bar{b} dz. \quad \square$$

Note that in formula (3.18), we can integrate by parts in z without any boundary contribution for $k \leq n$, because $\partial_z^j b = 0$ for $j = 0, \dots, n - 1$ on ∂I . Therefore

$$(3.19) \quad J_k = \left(\int_I a \partial_z^k \bar{b} dz \right) H_k[\alpha, p; \beta, q],$$

where

$$(3.20) \quad \begin{aligned} H_k[\alpha, p; \beta, q] &= \sum_{j+\ell=k} \int_0^\omega (-1)^j \left(T_0(\theta; \alpha + j, \partial_\theta) \varphi_j \cdot \bar{\psi}_\ell - \varphi_j \cdot T_0(\theta; -\beta + \ell, \partial_\theta) \bar{\psi}_\ell \right) d\theta \\ &- \sum_{j+\ell=k-1} \int_0^\omega (-1)^j \left(T_1(\theta) \varphi_j \cdot \bar{\psi}_\ell + \varphi_j \cdot T_1(\theta) \bar{\psi}_\ell \right) d\theta. \end{aligned}$$

As a consequence of the proof of Proposition 3.4 we have

$$(3.21) \quad \forall \alpha, \beta \in \mathfrak{A}, \quad \forall p, q, \quad \forall k \in \mathbb{N}, \quad H_k[\alpha, p; \beta, q] = \delta_{k,0} \delta_{\alpha,\beta} \delta_{p,q}.$$

Later on, we will use formula (3.21), and not Proposition 3.4, to extract the singularity coefficients of a true solution of problem (1.2).

4. Extraction of singularity coefficients. In this section, we first describe asymptotic expansions of the solution u of problem (1.2). The right-hand side f is $\mathcal{C}^\infty(\bar{\Omega})$, and we suppose in a preliminary step that $f \equiv 0$ in a neighborhood of the edge E . The expansions of u show edge singularity coefficients $a_{\alpha,p}$ along the edge E . We propose a method based on the duality formula (3.15) to determine these coefficients.

4.1. Expansion of the solution along the edge. The edge expansions are valid only away from the sides $G \times \partial I$. This is the reason why we introduce for any $\delta \in (0, 1)$ the subinterval

$$I_\delta = (-1 + \delta, 1 - \delta)$$

and consider the subdomains $G \times I_\delta$. We need the introduction of weighted spaces to describe the remainders in the expansions. For $\xi \in \mathbb{R}$, let

$$\mathcal{V}_\eta(G \times I_\delta) := \{v \in C^\infty(G \times I_\delta) \mid \forall \mathbf{m} \in \mathbb{N}^3, r^{-\eta+|\mathbf{m}|} \partial_{\mathbf{x}}^{\mathbf{m}} v \in L^\infty(G \times I_\delta)\}.$$

Then the following theorem holds; cf. [27].

THEOREM 4.1. *Let $\delta \in (0, 1)$ and $\eta > 0$ be given. Then for any $\alpha \in \mathfrak{A}$ such that $\operatorname{Re} \alpha \in (0, \eta)$ and for any $p \in \{1, \dots, p_\alpha\}$, there exists a unique coefficient $a_{\alpha,p} \in C^\infty(I_\delta)$ such that*

$$(4.1) \quad u - \sum_{\alpha, 0 < \operatorname{Re} \alpha < \eta} \sum_p S^n[\alpha, p; a_{\alpha,p}] \in \mathcal{V}_\eta(G \times I_\delta),$$

where $n = n(\alpha)$ is the smallest integer such that $\operatorname{Re} \alpha + n > \eta$.

Letting δ tend to 0, this clearly defines unique coefficients $a_{\alpha,p}$ in $C^\infty(I)$ such that for any δ (4.1) holds with $a_{\alpha,p}|_{I_\delta}$. But this *does not imply that* (4.1) holds in Ω , because in general the remainders on $G \times I_\delta$ depend on δ and their norms blow up as $\delta \rightarrow 0$. This is due to the presence of corner singularities at the corners $\mathbf{c}^\pm := (0, 0, \pm 1)$. We have to analyze these corner singularities in order to obtain uniform estimates in Ω .

4.2. Corner exponents. We describe the situation in a neighborhood of the corner \mathbf{c}^+ and particularize the notation by the superscript $+$. A similar situation holds for the other corner \mathbf{c}^- . Let K^+ be the infinite cone coinciding with Ω in a neighborhood of \mathbf{c}^+ . Let \mathbb{S}^+ denote the sphere of radius 1 centered at \mathbf{c}^+ , ρ^+ the distance to \mathbf{c}^+ , and ϑ^+ the coordinates on \mathbb{S}^+ . Thus (ρ^+, ϑ^+) are spherical coordinates centered at \mathbf{c}^+ . Finally, let S^+ denote the intersection $\mathbb{S}^+ \cap K^+$. The operator L can be written in these spherical coordinates as

$$L = (\rho^+)^{-2} \mathcal{L}^+(\vartheta^+; \rho^+ \partial_{\rho^+}, \partial_{\vartheta^+}),$$

which defines the Mellin symbol $\gamma \mapsto \mathfrak{L}^+(\gamma)$ of L at \mathbf{c}^+ , where $\mathfrak{L}^+(\gamma)$ is the operator $\phi \mapsto \mathcal{L}^+(\vartheta^+; \gamma, \partial_{\vartheta^+})\phi$ acting from $H_0^1(S^+)$ into $H^{-1}(S^+)$. We denote by \mathfrak{G}^+ the set of $\gamma \in \mathbb{C}$ such that $\mathfrak{L}^+(\gamma)$ is not invertible. We call these γ the *corner exponents*. We introduce the analogue of hypothesis (\mathfrak{H}_1) for \mathfrak{L}^+ :

$$(\mathfrak{H}_3) \quad \forall \gamma \in \mathfrak{G}^+, \quad \gamma \text{ is a pole of degree 1 of } (\mathfrak{L}^+)^{-1}.$$

For each $\gamma \in \mathfrak{G}^+$, we denote by $\phi[\gamma, q]$, $q = 1, \dots, q_\gamma$, a basis of $\ker \mathfrak{L}^+(\gamma)$.

We need a new family of weighted spaces: Let us introduce r^+ on S^+ as the distance to the corner ($r = 0, z = 0$) of S^+ corresponding to the edge E and extend it by homogeneity: $r^+(\mathbf{x}) = r^+(\vartheta^+(\mathbf{x}))$. Note that we have the equivalence

$$(4.2) \quad r^+(\mathbf{x}) \simeq r(\mathbf{x})/\rho^+(\mathbf{x}).$$

In the same way we define \tilde{r}^+ on S^+ as the distance to the two other corners of S^+ , ($r = 1, \theta = 0, z = 1$) and ($r = 1, \theta = \omega, z = 1$), and extend \tilde{r}^+ by homogeneity. We

define for $\xi > -\frac{1}{2}$ and $\eta > 0$

$$\mathcal{V}_{\xi, \eta}(\Omega^+) := \{v \in \mathcal{C}^\infty(\Omega^+) \mid \forall \mathbf{m} \in \mathbb{N}^3, (\rho^+)^{-\xi+|\mathbf{m}|} (r^+)^{-\eta+|\mathbf{m}|} (\tilde{r}^+)^{|\mathbf{m}|} \partial_{\mathbf{x}}^{\mathbf{m}} v \in L^\infty(\Omega^+)\},$$

with $\Omega^+ = G \times (0, 1)$. There holds the corner expansion for any fixed $\xi > -\frac{1}{2}$:

$$(4.3) \quad u - \sum_{\gamma, -1/2 < \text{Re } \gamma < \xi} \sum_q c_{\gamma, q} (\rho^+)^{\gamma} \phi[\gamma, q](\vartheta^+) \in \mathcal{V}_{\xi, 0}(\Omega^+),$$

where the coefficients $c_{\gamma, q}$ are complex numbers. Note that the remainder in (4.3) is *flat* with respect to the “distance” ρ^+ to the corner \mathbf{c}^+ and *not* with respect to the edge E . Thus, the expansions (4.1) and (4.3) give complementary and seemingly independent information about the structure of u .

In fact, we will use this result only to obtain the optimal corner regularity of u without splitting u into regular and singular parts at this corner. We define the set of exponents \mathfrak{G}^- attached to the corner c^- in a similar way as \mathfrak{G}^+ . We define ξ_1^\pm as

$$(4.4) \quad \xi_1^\pm = \min \{ \text{Re } \gamma \mid \gamma \in \mathfrak{G}^\pm \text{ and } \text{Re } \gamma > -\frac{1}{2} \}.$$

The choice $\xi = \xi_1^+$ is the best possible so that the corner expansion in (4.3) is empty. There holds

$$(4.5) \quad u \in \mathcal{V}_{\xi_1^+, 0}(\Omega^+) \quad \text{and} \quad u \in \mathcal{V}_{\xi_1^-, 0}(\Omega^-).$$

4.3. Edge expansion up to the corner. Relying on [14, Chap. 17] we can expand u along the edge E while taking its corner regularity into account. Near \mathbf{c}^+ the edge coefficients will themselves belong to weighted spaces of the type $\mathcal{V}_\xi(0, 1)$ on the half-edge $\{z \in (0, 1)\}$ (here ρ^+ coincides with $1 - z$),

$$\mathcal{V}_\xi(0, 1) := \{a \in \mathcal{C}^\infty(0, 1) \mid \forall m \in \mathbb{N}, (\rho^+)^{-\xi+m} \partial_{\rho^+}^m a \in L^\infty(0, 1)\},$$

and near c^- the coefficients will belong to a space $\mathcal{V}_\xi(-1, 0)$ where the weight function is $\rho^-(z) = 1 + z$ instead of ρ^+ .

THEOREM 4.2. *Let $\eta > 0$ be given. Then for any $\alpha \in \mathfrak{A}$ such that $\text{Re } \alpha \in (0, \eta)$ and any $p = 1, \dots, p_\alpha$, the coefficient $a_{\alpha, p}$ appearing in the splitting (4.1) belongs to $\mathcal{V}_{\xi_1^+ - \text{Re } \alpha}(0, 1)$ and there holds*

$$(4.6) \quad u - \sum_{\alpha, 0 < \text{Re } \alpha < \eta} \sum_p \chi(r^+) S^m[\alpha, p; a_{\alpha, p}] =: u_{\text{reg}, \eta}^+ \in \mathcal{V}_{\xi_1^+, \eta}(\Omega^+),$$

where χ is a smooth cut-off function which is 1 in a neighborhood of 0, $r^+ = r^+(\mathbf{x})$ is defined in (4.2), and $n = n(\alpha)$ is the smallest integer such that $\text{Re } \alpha + n > \eta$. Similarly, $a_{\alpha, p}|_{(-1, 0)}$ belongs to $\mathcal{V}_{\xi_1^- - \text{Re } \alpha}(-1, 0)$ and there holds

$$(4.7) \quad u - \sum_{\alpha, 0 < \text{Re } \alpha < \eta} \sum_p \chi(r^-) S^m[\alpha, p; a_{\alpha, p}] =: u_{\text{reg}, \eta}^- \in \mathcal{V}_{\xi_1^-, \eta}(\Omega^-).$$

4.4. Extraction of edge coefficients. Our main goal is the determination and the computation of the edge coefficients $a_{\alpha,p}$ —at least those corresponding to the smallest values of $\operatorname{Re} \alpha$. These coefficients are defined via the expansion (4.1), and a sharp estimate of both the coefficients and the remainder is given in Theorem 4.2. The method for extracting them is based on the use of the antisymmetric bilinear form $J[R](u, v)$ defined in (3.14), where v is chosen as $K^n[\beta, p; b]$ for a certain range of $\beta \in \mathfrak{A}$ and of test edge coefficients b . The choice of the order n will determine the order of the error, which is a positive power of R . We introduce a last technical hypothesis

$$(\mathfrak{H}_4) \quad \forall \alpha \in \mathfrak{A}, \operatorname{Re} \alpha \geq 0, \quad \xi_1^+ - \operatorname{Re} \alpha \notin \mathbb{N}, \quad \xi_1^- - \operatorname{Re} \alpha \notin \mathbb{N}.$$

The main result of our work is the following.

THEOREM 4.3. *Let u be the solution of problem (1.2) with a smooth right-hand side f , which is zero in a neighborhood of the edge E . We assume the hypotheses (\mathfrak{H}_1) – (\mathfrak{H}_4) . The function u admits the edge expansion (4.1) for all $\delta > 0$. Let $\beta \in \mathfrak{A}$ with $\operatorname{Re} \beta > 0$. We fix an integer $n \geq 0$ such that*

$$(4.8) \quad n \geq \operatorname{Re} \beta - \xi_1 - 1 \quad \text{with} \quad \xi_1 = \min\{\xi_1^+, \xi_1^-\},$$

where we recall that ξ_1^+ defined in (4.4) is attached to the corner \mathbf{c}^+ and ξ_1^- is its analogue for the corner \mathbf{c}^- . Let m be an integer $m \geq n$ and finally let $b \in \mathcal{C}^m(\bar{I})$ be such that $\partial_z^j b(\pm 1) = 0$ for all $j = 0, \dots, n - 1$. Then there holds

$$(4.9) \quad J[R](u, K^m[\beta, p; b]) = \int_I a_{\beta,p}(z) \bar{b}(z) \, dz + \mathcal{O}\left(R^{\min\{n+\xi_1, m+\eta_1\} - \operatorname{Re} \beta + 1}\right)$$

as $R \rightarrow 0$, where

$$(4.10) \quad \eta_1 = \min\{\operatorname{Re} \alpha \mid \alpha \in \mathfrak{A} \text{ and } \operatorname{Re} \alpha > 0\}.$$

Before starting the proof, we give a corollary of identity (3.21). For this, we first introduce the decomposition of the bilinear form $J[R]$ according to the splitting (3.7) of the radial traction T :

$$J^0[R](u, v) := \int_{\Gamma_R} (T_0 u \cdot \bar{v} - u \cdot T_0 \bar{v}) R^{-1} \, d\sigma = \int_I \int_0^\omega (T_0 u \cdot \bar{v} - u \cdot T_0 \bar{v})|_{r=R} \, d\theta \, dz$$

and

$$J^1[R](u, v) := \int_{\Gamma_R} (T_1 u \cdot \bar{v} - u \cdot T_1 \bar{v}) \, d\sigma = \int_I \int_0^\omega (T_1 u \cdot \bar{v} - u \cdot T_1 \bar{v})|_{r=R} \, R \, d\theta \, dz.$$

LEMMA 4.4. *Let $\alpha, \beta \in \mathfrak{A}$. Let $m \in \mathbb{N}$ and integers $0 \leq n \leq m, 0 \leq k \leq m$. Let $b \in \mathcal{C}^m(\bar{I})$ such that $\partial_z^j b(\pm 1) = 0$ for all $j = 0, \dots, n - 1$. Let $a \in \mathcal{V}_\xi(-1, 1)$. If $\xi + n - k + 1 > 0$, then*

$$\begin{aligned} & \sum_{j+\ell=k} J^0[R](\partial_z^j a \Phi_j[\alpha, q], \partial_z^\ell b \Psi_\ell[\beta, p]) \\ & + \sum_{j+\ell=k-1} J^1[R](\partial_z^j a \Phi_j[\alpha, q], \partial_z^\ell b \Psi_\ell[\beta, p]) = \delta_{k,0} \delta_{\alpha,\beta} \delta_{p,q} \int_I a(z) \bar{b}(z) \, dz. \end{aligned}$$

This lemma is merely a consequence of identity (3.21). Indeed, the assumptions about a and b ensure that (i) all integrals in z are convergent, and (ii) integrations by

parts in z (to have all derivatives on b) do not produce any boundary contribution. Therefore we can separate the integrals over I and $(0, \omega)$ as in (3.19). The integrals over $(0, \omega)$ are zero (or 1) thanks to (3.21), which correspondingly yields the lemma.

Proof of Theorem 4.3. Relying on the decompositions (4.6)–(4.7) of u , we split the integral $J[R](u, K^m[\beta, p; b])$ into several pieces, $I_0 + I_1^+ + I_2^+ + I_1^- + I_2^- + I_3$, and estimate each of them.

- We first assume that $m > n + \xi_1 - \eta_1$.

(A) We define I_0 as

$$I_0 = \sum_{\substack{\alpha, q, k \\ \xi_1 - \operatorname{Re} \alpha + n - k + 1 > 0}} \left(\sum_{j+\ell=k} J^0[R](\partial_z^j a_{\alpha, q} \Phi_j[\alpha, q], \partial_z^\ell b \Psi_\ell[\beta, p]) + \sum_{j+\ell=k-1} J^1[R](\partial_z^j a_{\alpha, q} \Phi_j[\alpha, q], \partial_z^\ell b \Psi_\ell[\beta, p]) \right),$$

where the coefficients $a_{\alpha, q}$ are those of expansion (4.6). The assumptions of Lemma 4.4 are fulfilled because of the following:

- (a) The inequality $\xi_1 - \operatorname{Re} \alpha + n - k + 1 > 0$ implies that $k < \xi_1 - \operatorname{Re} \alpha + n + 1$, which is $\leq n + \xi_1 - \eta_1$; since we have assumed that $m > n + \xi_1 - \eta_1$, then $k \leq m$.
- (b) By Theorem 4.2, $a_{\alpha, q}$ belongs to the weighted space $\mathcal{V}_{\xi_1^+ - \operatorname{Re} \alpha}(0, 1)$ in the part of the edge which belongs to Ω^+ , and similarly in Ω^- ; therefore the inequality $\xi_1 - \operatorname{Re} \alpha + n - k + 1 > 0$ is the assumption $\eta + n - k + 1 > 0$ of Lemma 4.4.

Moreover, the assumption $n \geq \operatorname{Re} \beta - \xi_1 - 1$ implies that the triple $(\alpha = \beta, q = p, k = 0)$ belongs to the sum defining I_0 . Therefore

$$I_0 = \int_I a_{\beta, p}(z) \bar{b}(z) \, dz.$$

(B) We define I_1^+ as

$$I_1^+ = \sum_{\substack{\alpha, q, k \\ \xi_1^+ - \operatorname{Re} \alpha + n - k + 1 > 0}} \left(\sum_{j+\ell=k} J^0[R](\chi(r^+) - 1) \partial_z^j a_{\alpha, q} \Phi_j[\alpha, q], \partial_z^\ell b \Psi_\ell[\beta, p]) + \sum_{j+\ell=k-1} J^1[R](\chi(r^+) - 1) \partial_z^j a_{\alpha, q} \Phi_j[\alpha, q], \partial_z^\ell b \Psi_\ell[\beta, p]) \right).$$

Let us define z^+ as $1 - z$. The domain of integration of the terms in I_1^+ is $\Gamma_R \cap \operatorname{supp}(\chi(r^+) - 1)$ and is contained in a set of the form

$$\{\mathbf{x} \in \mathbb{R}^3 \mid r = R, \theta \in (0, \omega), z^+ \in (0, cR)\},$$

where c is a positive constant.

Each term in I_1^+ can be estimated by a product of three terms:

- (i) an integral in z^+ over $(0, cR)$ of a function depending on z^+ but not on R or θ ;
- (ii) an integral in θ over $(0, \omega)$ of a function depending on θ but not on R or z^+ ;
- (iii) a power of R corresponding to the restriction on Γ_R of a power of r .

We observe the following:

(i) The integral over $(0, cR)$ is $\int_0^{cR} (z^+)^{\xi_+^1 - \text{Re } \alpha + n - k} dz^+$, which is $\mathcal{O}(R^{\xi_+^1 - \text{Re } \alpha + n - k + 1})$ since $\xi_+^1 - \text{Re } \alpha + n - k + 1 > 0$.

(ii) The integral over $(0, \omega)$ does not depend on R .

(iii) The power of R is $R^{\text{Re } \alpha - \text{Re } \beta + k}$.

Therefore

$$I_1^+ = \mathcal{O}\left(R^{\xi_+^1 + n - \text{Re } \beta + 1}\right).$$

The corresponding part I_1^- in the neighborhood of \mathbf{c}^- has a similar bound.

(C) We define I_2^+ as

$$I_2^+ = \sum_{\substack{\alpha, q, j, \ell \\ \xi_+^1 - \text{Re } \alpha + n - j - \ell + 1 < 0 \\ \ell \leq m, \text{Re } \alpha + j < n + \xi_+^1 + 1}} \left(\sum_{j+\ell=k} J_+^0[R](\chi(r^+) \partial_z^j a_{\alpha, q} \Phi_j[\alpha, q], \partial_z^\ell b \Psi_\ell[\beta, p]) \right. \\ \left. + \sum_{j+\ell=k-1} J_+^1[R](\chi(r^+) \partial_z^j a_{\alpha, q} \Phi_j[\alpha, q], \partial_z^\ell b \Psi_\ell[\beta, p]) \right),$$

where J_+^0 and J_+^1 are the contributions over Ω^+ of J^0 and J^1 .

As for I_1^+ , each term of I_2^+ can be estimated by the product of three terms (i)–(iii). The only difference is that the integral (i) in z^+ is over $(cR, 1)$ instead of $(0, cR)$ and is equal to $\int_{cR}^1 (z^+)^{\xi_+^1 - \text{Re } \alpha + n - k} dz^+$, which is still $\mathcal{O}(R^{\xi_+^1 - \text{Re } \alpha + n - k + 1})$ since $\xi_+^1 - \text{Re } \alpha + n - k + 1 < 0$. The power (iii) of R is the same; thus we obtain, as above, that

$$I_2^+ = \mathcal{O}\left(R^{\xi_+^1 + n - \text{Re } \beta + 1}\right).$$

(D) We set $\eta := n + \xi_+^1 + 1$. We check that

$$I_0 + I_1^+ + I_1^- + I_2^+ + I_2^- = \sum_{\substack{\alpha, q, j \\ \text{Re } \alpha + j < \eta}} J[R](\chi(r^+) \partial_z^j a_{\alpha, q} \Phi_j[\alpha, q], K^m[\beta, p; b]).$$

But according to Theorem 4.2

$$u_{\text{reg}, \eta}^+ := u - \sum_{\substack{\alpha, q, j \\ \text{Re } \alpha + j < \eta}} \chi(r^+) \partial_z^j a_{\alpha, q} \Phi_j[\alpha, q] \in \mathcal{V}_{\xi_+^1, \eta}(\Omega^+),$$

and similarly for the other corner. Therefore it remains to estimate

$$I_3 := J[R](u_{\text{reg}, \eta}^+, K^m[\beta, p; b])$$

and, more precisely, each contribution $J[R](u_{\text{reg}, \eta}^+, \partial_z^\ell b \Psi_\ell)$ for $\ell = 0, \dots, m$. Since $u_{\text{reg}, \eta}^+$ belongs to $\mathcal{V}_{\xi_+^1, \eta}(\Omega^+)$,

$$u_{\text{reg}, \eta}^+ = \mathcal{O}\left((\rho^+)^{\xi_+^1} (r^+)^\eta\right) = \mathcal{O}\left((\rho^+)^{\xi_+^1 - \eta} r^\eta\right) \quad \text{and} \quad \nabla u_{\text{reg}, \eta}^+ = \mathcal{O}\left((\rho^+)^{\xi_+^1 - \eta} r^{\eta-1}\right).$$

For the bounding of $J[R](u_{\text{reg}, \eta}^+, \partial_z^\ell b \Psi_\ell)$, we split the integral over Γ_R into (a) the contribution on $z^+ \in (0, R)$, and (b) the contribution on $z^+ \in (R, 1)$, and we estimate each piece by a product of three terms as we did before.

- (a) When $z^+ \in (0, R)$, the distance ρ^+ is equivalent to R on Γ_R . Therefore the weight over $u_{\text{reg},\eta}^+$ is equivalent to $R^{\xi_1^+}$ in that region. Part (i) is the integral $\int_0^R (z^+)^{n-\ell} dz^+ = \mathcal{O}(R^{n-\ell+1})$, and the power (iii) of R is $R^{\xi_1^+ - \text{Re } \beta + \ell}$. Their product is $R^{n+\xi_1^+ - \text{Re } \beta + 1}$.
- (b) When $z^+ \in (R, 1)$, the distance ρ^+ is equivalent to z^+ on Γ_R . Therefore the weight over $u_{\text{reg},\eta}^+$ is equivalent to $(z^+)^{\xi_1^+ - \eta} r^\eta$ in that region. Part (i) is the integral $\int_R^1 (z^+)^{\xi_1^+ - \eta + n - \ell} dz^+ = \mathcal{O}(R^{\xi_1^+ - \eta + n - \ell + 1})$ (since $\xi_1^+ - \eta + n - \ell + 1 < 0$), and the power (iii) of R is $R^{\eta - \text{Re } \beta + \ell}$. The product of both is $R^{\xi_1^+ + n + 1 - \text{Re } \beta}$.

Gathering all the previous results of parts (A)–(D), we obtain formula (4.9) in the case $m > n + \xi_1 - \eta_1$.

- When $m < n + \xi_1 - \eta_1$, we follow the same lines with the corresponding changes:

For I_0 we reduce the sum by the extra condition that $k \leq m$, and the same for I_1^+ . The conclusions are still the same. For I_2^+ the sum is augmented by the set of (α, j, ℓ) such that $\xi_1^+ - \text{Re } \alpha + n - j - \ell + 1 > 0$ and $j + \ell > m$. The new terms do not satisfy the same estimates as the old ones since the corresponding contribution (i) in z^+ is now $\mathcal{O}(1)$. As the power (iii) of R is still $R^{\text{Re } \alpha - \text{Re } \beta + j + \ell}$, we obtain that

$$I_2^+ = \min \left\{ \mathcal{O}(R^{\xi_1^+ + n - \text{Re } \beta + 1}), \mathcal{O}(R^{\text{Re } \alpha - \text{Re } \beta + j + \ell}) \right\},$$

where the min is taken over (α, j, ℓ) such that $\xi_1^+ - \text{Re } \alpha + n - j - \ell + 1 > 0$ and $j + \ell > m$. The minimum of $\text{Re } \alpha + j + \ell$ is attained for $\alpha = \beta_1$ and $j + \ell = m + 1$, whence

$$I_2^+ = \mathcal{O}(R^{m_1 - \text{Re } \beta + m + 1}).$$

We have proved formula (4.9) in the case $m < n + \xi_1 - \eta_1$. □

Remark 4.5. (i) Formula (4.9) is, of course, still valid if hypotheses (\mathfrak{H}_1) – (\mathfrak{H}_4) are only assumed to hold for the exponents which are used in the proof, namely, $\text{Re } \beta < \eta = n + \xi_1 + 1$ for (\mathfrak{H}_1) , (\mathfrak{H}_2) , and (\mathfrak{H}_4) and $\text{Re } \gamma = \xi_1^+$ for (\mathfrak{H}_3) .

(ii) If we discard hypotheses (\mathfrak{H}_3) and (\mathfrak{H}_4) , we can still prove a formula like (4.9), up to the possible multiplication of the remainder by $|\log^M R|$ for some integer M .

(iii) We still obtain formula (4.9) if we relax the assumption on the right-hand side so that f is no longer supposed to be zero in the neighborhood of the edge, but only flat up to a specified order, in relation to what is needed in the proof of (4.9): it suffices that f belongs to the weighted spaces $\mathcal{V}_{\xi_1-2, \eta-2}(\Omega^+)$ and $\mathcal{V}_{\xi_1-2, \eta-2}(\Omega^-)$, with ξ_1 defined in (4.8) and $\eta = n + \xi_1 + 1$. Then the edge expansion up to the corner (4.6) still holds with such a right-hand side, which makes part (D) of the proof of (4.9) still valid.

Remark 4.6. The assumptions about the test edge coefficients b can be slightly relaxed.

(i) Instead of the boundary conditions $\partial_z^j b(\pm 1) = 0$ for any $j = 0, \dots, n - 1$, we may assume that $(1 - z)^{-n+j}(z + 1)^{-n+j} \partial_z^j b \in L^\infty(I)$ for $j \leq m$, and the statement of Theorem 4.3 can be extended to *noninteger* n .

(ii) We may assume that b is only $\mathcal{C}^{m-1}(\bar{I})$ globally and piecewise \mathcal{C}^m on a finite partition of I .

5. A wider range of applications for quasi-dual methods. We extend the results of Theorem 4.3 to any edge of a general polyhedron and discuss the case of cracks (where $\omega = 2\pi$). We also evaluate the limitation of the convergence rate in R when the right-hand side is not flat along the edge.

5.1. The domain. By a slight modification we can adapt our method to the determination of edge singularities along any edge of a three-dimensional polyhedron, that is, a domain Ω with plane faces and, therefore, straight edges.

Let E be an edge of Ω . E is an open segment whose end points \mathbf{c}^+ and \mathbf{c}^- are corners of Ω . We choose cylindrical coordinates (r, θ, z) adapted to Ω around E :

$$E = \{ \mathbf{x} \sim (r, \theta, z) \mid r = 0, z \in (-\frac{h}{2}, \frac{h}{2}) \},$$

where h is the length of E . There exists a conical neighborhood¹ Θ of E such that

$$\Omega \cap \Theta = \{ \mathbf{x} \sim (r, \theta, z) \mid r \in (0, 1), \omega \in (0, \omega), z \in (-\frac{h}{2}, \frac{h}{2}) \} \cap \Theta,$$

where ω is the opening of Ω along the edge E .

We still define, for any $R < 1$, the internal cylinder Γ_R as

$$\Gamma_R = \{ \mathbf{x} \sim (r, \theta, z) \mid r = R, \omega \in (0, \omega), z \in (-\frac{h}{2}, \frac{h}{2}) \}.$$

But it may happen that even for small R , Γ_R is not included in Ω . Then we define the reduced internal cylinder $\check{\Gamma}_R$ as

$$\check{\Gamma}_R = \{ \mathbf{x} \sim (r, \theta, z) \mid r = R, \omega \in (0, \omega), z \in (-\frac{h}{2} + kR, \frac{h}{2} - kR) \},$$

where $k > 0$ defines the conical neighborhood Θ . In other words, for any $R \leq R_0$, $\check{\Gamma}_R = \Gamma_R \cap \Theta$.

On the same model as (3.14), we define

$$(5.1) \quad \check{J}[R](u, v) := \int_{\check{\Gamma}_R} (Tu \cdot \bar{v} - u \cdot T\bar{v}) \, d\sigma = \int_{-\frac{h}{2} + kR}^{\frac{h}{2} - kR} \int_0^\omega (Tu \cdot \bar{v} - u \cdot T\bar{v}) \Big|_{r=R} R \, d\theta \, dz.$$

Then defining the sets \mathfrak{G}^\pm of corner exponents at \mathbf{c}^\pm as before, but now on the polyhedral cones K^\pm coinciding with Ω in neighborhoods of \mathbf{c}^\pm , and defining ξ_1^\pm in the same way, we have expansions² (4.6)–(4.7), and there holds, with the same assumptions as in Theorem 4.3,

$$(5.2) \quad \check{J}[R](u, K^m[\beta, p; b]) = \int_{-\frac{h}{2}}^{\frac{h}{2}} a_{\beta, p}(z) \bar{b}(z) \, dz + \mathcal{O} \left(R^{\min\{n+\xi_1, m+\eta_1\} - \text{Re } \beta + 1} \right).$$

The proof follows exactly the same steps as the proof of (4.9). The parts I_0, I_1^\pm , and I_2^\pm are still defined by integrals over Γ_R . We modify only part (D), noting that, thanks to the condition on the support of χ , the expansion (4.6) now gives

$$\check{J}[R](u, K^m[\beta, p; b]) = \check{J}[R](u_{\text{reg}, \eta}^+, K^m[\beta, p; b]) + I_0 + I_1^+ + I_1^- + I_2^+ + I_2^-.$$

The conclusion follows by the same arguments as before.

¹In cylindrical coordinates, Θ has the form

$$\Theta = \{ \mathbf{x} \sim (r, \theta, z) \mid r \in (0, R_0), \omega \in (0, \omega), z \in (-\frac{h}{2} + kr, \frac{h}{2} - kr) \},$$

with a $k > 0$ and $R_0 > 0$.

²With the cut-off function χ chosen so that in the cylinder $r \leq R_0$, the support of $\mathbf{x} \mapsto \chi(r^\pm)$ is contained in the conical neighborhood Θ . The subdomains Ω^+ and Ω^- correspond to the regions $z > 0$ and $z < 0$, respectively.

5.2. In the presence of cracks. We now consider the case where the opening ω is equal to 2π . This means that the model domain Ω is the cylinder of radius 1 with an internal boundary formed by the plane rectangle

$$\Sigma = \{\mathbf{x} \in \mathbb{R}^3 \mid x \in (0, 1), y = 0, z \in I\}.$$

This case is in principle included in our analysis. But the special situation of the singularity exponents prevents hypothesis (\mathfrak{H}_2) from being satisfied: By the result of [10], the set \mathfrak{A} of singular exponents is included in the set of half-integers and, moreover,

$$(5.3) \quad \forall \bar{j} \in \mathbb{N}, \quad \dim \ker \mathfrak{M}_0(\tfrac{1}{2} + \bar{j}) = N,$$

where we recall that N is the size of the system L . But our method can still be applied in this case! We are going to explain why.

The first place where we use (\mathfrak{H}_2) is for the definition of the shadow singularities $\Phi_j[\alpha, p]$. The general theory gives that $\Phi_j[\alpha, p]$ can be found in the form of a finite sum of the form $r^{\alpha+j} \sum \log^q r \varphi_{j,q}(\theta)$. But in this situation of cracks, it is proved in [11] that the logarithmic terms are absent. But still, the solution of (2.8), though existing, is not unique. This circumstance will help in the second place where we use (\mathfrak{H}_2) .

We used (\mathfrak{H}_2) to prove (3.21), in particular that $H_k[\alpha, p; \beta, q] = 0$ for all α and β in \mathfrak{A} when $k \neq 0$.

LEMMA 5.1. *For all $\bar{j} \in \mathbb{N}$, $p = 1, \dots, N$, and $j \geq 1$ let the singularities $\Phi_0[\frac{1}{2} + \bar{j}, p]$ and their shadows $\Phi_j[\frac{1}{2} + \bar{j}, p]$ be fixed. The dual singularities $\Psi_0[\frac{1}{2} + \bar{\ell}, q]$ are still determined according to Lemma 3.2, and there exists a choice of the shadows $\Psi_\ell[\frac{1}{2} + \bar{\ell}, q]$ such that there holds (cf. (3.20) and (3.21))*

$$(5.4) \quad \forall \bar{j}, \bar{\ell} \in \mathbb{N}, \quad \forall p, q \leq N, \quad \forall k > 0, \quad H_k[\tfrac{1}{2} + \bar{j}, p; \tfrac{1}{2} + \bar{\ell}, q] = 0.$$

Proof. By the proof of Proposition 3.4, we know that for any choice of the $\Psi_\ell[\beta, q]$, the identity $H_k[\alpha, p; \beta, q] = 0$ holds as soon as $\alpha - \beta + k \neq 0$, i.e., in our case, when $\frac{1}{2} + \bar{j} - \frac{1}{2} - \bar{\ell} + k \neq 0$. Thus it remains to prove (5.4) when $\bar{j} - \bar{\ell} + k = 0$.

Let $\bar{\ell}$ and q be fixed. The proof uses induction over k . For $k = 1$, $\bar{j} = \bar{\ell} - 1$. Let us fix a particular solution $\check{\psi}_1[\frac{1}{2} + \bar{\ell}, q]$ of (3.12). Any solution of (3.12) is the sum of $\check{\psi}_1[\frac{1}{2} + \bar{\ell}, q]$ and of an element of $\ker \mathfrak{M}_0(-\frac{1}{2} - \bar{\ell} + 1) = \ker \mathfrak{M}_0(-\frac{1}{2} - \bar{j})$. A basis of this kernel is the set of $\psi_0[\frac{1}{2} + \bar{j}, p']$, $p' = 1, \dots, N$. Therefore $H_1[\frac{1}{2} + \bar{j}, p; \frac{1}{2} + \bar{\ell}, q]$ is the sum of a fixed contribution and of a linear combination of the contributions of the $\psi_0[\frac{1}{2} + \bar{j}, p']$, i.e., of $H_0[\frac{1}{2} + \bar{j}, p; \frac{1}{2} + \bar{j}, p']$. By Lemma 3.2, we can determine elements of the kernel $\ker \mathfrak{M}_0(-\frac{1}{2} - \bar{j})$ so that $H_1[\frac{1}{2} + \bar{j}, p; \frac{1}{2} + \bar{\ell}, q] = 0$ for all $p = 1, \dots, N$.

For a general k , we assume that the $\Psi_\ell[\frac{1}{2} + \bar{\ell}, q]$ are determined for $\ell < k$ and have to prove (5.4) for $\bar{j} = \bar{\ell} - k$. We isolate the contribution $j = 0, \ell = k$ in H_k , and the proof is similar to the case $k = 1$. \square

5.3. The right-hand side. Let us consider now a standard smooth right-hand side $f \in \mathcal{C}^\infty(\bar{\Omega})$. Then f belongs to the weighted spaces $\mathcal{V}_{0,0}(\Omega^+)$ and $\mathcal{V}_{0,0}(\Omega^-)$. With

$$(5.5) \quad \xi_0^+ = \min\{\xi_1^+, 2\} \quad \text{and} \quad \xi_0^- = \min\{\xi_1^-, 2\},$$

there holds, for $\eta = 2$,

$$(5.6) \quad f \in \mathcal{V}_{\xi_0^+ - 2, \eta - 2}(\Omega^+) \quad \text{and} \quad f \in \mathcal{V}_{\xi_0^- - 2, \eta - 2}(\Omega^-).$$

Thus a general smooth interior right-hand side alters the asymptotics of the solution only in the region of exponents $\operatorname{Re} \alpha \geq 2$ and $\operatorname{Re} \gamma \geq 2$. The corresponding parts in the asymptotics of u (either polynomial or singular) are no longer orthogonal in the sense of the bilinear form $J[R]$ versus the standard singularities associated with a zero (or flat) right-hand side.

In connection with Remark 4.5(iii), we see that in order to take (5.6) into account, we first have to replace ξ_1 by $\xi_0 := \min\{\xi_0^+, \xi_0^-\}$ in the statement of Theorem 4.3 and investigate the consequences on the estimates of the limitation $\eta = 2$.

We assume that $m > n + \xi_0 - \eta_1$. We make changes in the general proof of Theorem 4.3 in the same spirit as at the end of this proof: For I_0 we reduce the sum by the extra condition that $\operatorname{Re} \beta + k < 2$, and the same for I_1^\pm . Thus we require that $\operatorname{Re} \alpha < 2$ so that the triple $(\beta = \alpha, q = p, k = 0)$ belongs to the sum defining I_0 . The conclusions are still the same.

For I_2^+ the sum is augmented by the set of (β, q, j, ℓ) such that $\xi_1^+ - \operatorname{Re} \beta + n - j - \ell + 1 > 0$ and $\operatorname{Re} \beta + j + \ell \geq 2$. The new terms do not satisfy the same estimates as the old ones since the corresponding contribution (i) in z^+ is now $\mathcal{O}(1)$. As the power (iii) of R is still $R^{\operatorname{Re} \beta - \operatorname{Re} \alpha + j + \ell}$, we obtain

$$I_2^+ = \min \left\{ \mathcal{O}(R^{\xi_1^+ + n - \operatorname{Re} \alpha + 1}), \mathcal{O}(R^{\operatorname{Re} \beta - \operatorname{Re} \alpha + j + \ell}) \right\},$$

where the min is taken over (β, j, ℓ) such that $\xi_1^+ - \operatorname{Re} \beta + n - j - \ell + 1 > 0$ and $\operatorname{Re} \beta + j + \ell \geq 2$.

We have also to consider I_3 anew with the constraint that $\eta = 2$. Part (a) of the estimate is the same, but concerning part (b), we now have to deal with the possibility that $\xi_0^+ - \eta + n + 1 = \xi_0^+ - 2 + n + 1$ may be ≥ 0 . In this case, the contribution (i) is $\mathcal{O}(1)$ and the contribution (iii) is $R^{\eta - \operatorname{Re} \alpha} = R^{2 - \operatorname{Re} \alpha}$.

Let $Q[R](u, K^m[\alpha, p; b])$ be the remainder $J[R](u, K^m[\alpha, p; b]) - \int_I a_{\alpha, p}(z) \bar{b}(z) dz$.

THEOREM 5.2. *Let u be the solution of problem (1.2) with a smooth right-hand side $f \in C^\infty(\bar{\Omega})$. We assume the hypotheses (\mathfrak{H}_1) – (\mathfrak{H}_4) . Let $\alpha \in \mathfrak{A}$ with $\operatorname{Re} \alpha \in (0, 2)$. We fix an integer $n \geq 0$ such that*

$$(5.7) \quad n \geq \operatorname{Re} \alpha - \xi_0 - 1.$$

Let m be an integer $m \geq n$ and let $b \in C^m(\bar{I})$ be such that $\partial_z^j b(\pm 1) = 0$ for all $j = 0, \dots, n - 1$. Then there holds

$$(5.8) \quad Q[R](u, K^m[\alpha, p; b]) = \mathcal{O}\left(R^{\min\{1, n + \xi_1, m + \eta_1\} - \operatorname{Re} \alpha + 1}\right).$$

Remark 5.3. If f is zero on the edge E , then f belongs to $\mathcal{V}_{1,1}(\Omega^\pm)$ and the above statement can be improved by replacing everywhere 2 by 3, including in the definition (5.5) of ξ_0^\pm , and we obtain the following estimate for the remainder:

$$(5.9) \quad Q[R](u, K^m[\alpha, p; b]) = \mathcal{O}\left(R^{\min\{2, n + \xi_1, m + \eta_1\} - \operatorname{Re} \alpha + 1}\right).$$

5.4. Other boundary conditions. In a way similar to that described in detail for Dirichlet boundary conditions, we can treat other self-adjoint boundary conditions such as Neumann conditions or mixed conditions in several forms, i.e., Dirichlet on certain faces and Neumann on the others, or of mixed type for systems, where, for example, in elasticity some components of the displacement are prescribed to 0 and the complementing components of the traction are also prescribed.

We may also consider transmission conditions based on a coercive bilinear form B with piecewise constant coefficients.

Once the correct Mellin symbols \mathfrak{M}_0 and \mathfrak{L}^\pm are defined, we consider their respective spectra \mathfrak{A} and \mathfrak{G}^\pm and everything works in the same way, mutatis mutandis. But we have to emphasize that the sets of exponents \mathfrak{A} and \mathfrak{G}^\pm may systematically contain (small) integers. For example, if we consider a Neumann problem, 0 always belongs to \mathfrak{A} and \mathfrak{G}^\pm , which implies that $\alpha_1 = 0$ (and, in general, $\xi_1 = 0$), though this zero exponent corresponds to a “singular function” Φ_0 which is constant.

Also the consideration of nonzero boundary data in the neighborhood of the edge would introduce more perturbation in the orthogonality relations between the asymptotics of the solution and the standard singularities associated with a zero right-hand side.

6. Other methods and formulas: A comparison. Inspired by [26] and [20] we can provide other families of formulas for the determination of the edge coefficients. We present them and then compare them with each other. All of them are valid in the extended framework of polyhedral domains as in section 5.1.

6.1. Pointwise dual formulas. Adapting [26] we find the formula, valid for any solution u of (1.2) with smooth $Lu = f$, sufficiently flat near the edge E : For each fixed $z_0 \in I$,

$$(6.1) \quad a_{\alpha,p}(z_0) = \int_{\Omega} Lu \cdot \overline{K}_{z_0}[\alpha, p] \, dx \, dy \, dz.$$

The three-dimensional dual function $(x, y, z) \mapsto K_{z_0}[\alpha, p](x, y, z)$ is defined as

$$K_{z_0}[\alpha, p] := \Psi_{z_0}^{3D}[\alpha, p] - X_{z_0}[\alpha, p],$$

where the following hold:

1. $\Psi_{z_0}^{3D}[\alpha, p]$ is a dual three-dimensional “corner” singularity at $(0, 0, z_0)$ considered the vertex of a cone: With ρ_0 the distance to the point $(0, 0, z_0)$, and ϑ_0 the corresponding spherical coordinates, $\Psi_{z_0}^{3D}[\alpha, p]$ has the form

$$\Psi_{z_0}^{3D}[\alpha, p](\rho_0, \vartheta_0) = \rho_0^{-1-\bar{\alpha}} \psi[\alpha, p](\vartheta_0)$$

and satisfies on the infinite wedge W_I coinciding with Ω in the conical neighborhood Θ

$$\begin{cases} LX_{z_0}^{3D}[\alpha, p] = 0 & \text{in } W_I, \\ \Psi_{z_0}^{3D}[\alpha, p] = 0 & \text{on } \partial W_I. \end{cases}$$

It does not belong to H^1 in any neighborhood of z_0 due to its strong singularity in $\rho_0^{-1-\bar{\alpha}}$. The spherical pattern ψ depends only on the wedge W_I and the operator L , but not on the particular point z_0 since we have supposed that the operator has constant coefficients.

2. $X_{z_0}[\alpha, p]$ is the correction in $H^1(G)$, solution of

$$(6.2) \quad \begin{cases} LX_{z_0}[\alpha, p] = 0 & \text{in } \Omega, \\ X_{z_0}[\alpha, p] = \Psi_{z_0}^{3D}[\alpha, p]|_{\partial\Omega} & \text{on } \partial\Omega. \end{cases}$$

Note that X_{z_0} strongly depends on z_0 , because the trace of $\Psi_{z_0}^{3D}[\alpha, p]$ on $\partial\Omega$ depends on z_0 .

6.2. Global dual formulas. In the same spirit as formulas (6.1)–(6.2), we can also obtain exact formulas for moments of the coefficients: For test functions $b \in \mathcal{C}_0^\infty(I)$ (or, more generally, b as in Theorem 4.3 with n large enough)

$$(6.3) \quad \int_{-1}^1 a_{\alpha,p}(z) b(z) \, dz = \int_{\Omega} Lu \cdot \overline{K}_b[\alpha, p] \, dx \, dy \, dz.$$

Here $K_b[\alpha, p] := K^m[\alpha, p; b] - X_b[\alpha, p]$, where $K^m[\alpha, p; b]$ is defined in (3.11) with $m > \operatorname{Re} \alpha - 1$ (i.e., so that $LK^m[\alpha, p; b]$ belongs to $H^{-1}(\Omega)$; see (3.13)) and $X_b[\alpha, p]$ is the correction in $H^1(G)$, solution of

$$(6.4) \quad \begin{cases} LX_b[\alpha, p] = LK^m[\alpha, p; b] & \text{in } \Omega, \\ X_b[\alpha, p] = K^m[\alpha, p; b]|_{\partial\Omega} & \text{on } \partial\Omega. \end{cases}$$

Compare with [20], where the case $L = \Delta$ with $m = 0$ is considered.

An alternative to (6.3) in the spirit of [15] is the following mixed formula:

$$(6.5) \quad \int_{-1}^1 a_{\alpha,p}(z) b(z) \, dz = \int_{\Omega} Lu \cdot \chi \overline{K}^m[\alpha, p; b] - u \cdot L(\chi \overline{K}^m[\alpha, p; b]) \, dx \, dy \, dz.$$

Here the cut-off χ can be taken as in the expansions (4.6)–(4.7), i.e., $\chi(\mathbf{x}) = \chi(r^+)$ in Ω^+ and $\chi(\mathbf{x}) = \chi(r^-)$ in Ω^- . Simpler cut-off can be used if Ω contains a cylinder of the form $\{\mathbf{x}, r < r_0, 0 < \theta < \omega, z \in I\}$: then $\chi = \chi(r)$ with $\chi(r) \equiv 1$ for $r < r_0/2$ and $\equiv 0$ for $r \geq r_0$.

6.3. Comparison. Formula (6.1) yields exact pointwise values for the edge coefficient, provided the right-hand side is smooth enough to ensure the continuity of the coefficient and flat enough to cancel any Taylor part of degree $\leq \operatorname{Re} \alpha$ in the solution u . This formula makes use of the right-hand side only and does not need the computation of u . But its main drawback is its own computation. The determination of the dual spherical pattern $\psi[\alpha, p]$ is seldom explicit and difficult in general: In addition to the Laplace operator, this is done only for the Lamé system under Neumann boundary conditions for a crack situation ($\omega = 2\pi$); see [30]. Moreover the solution of the three-dimensional problem (6.2) is necessary for each value of z_0 where we want to have the value of the coefficient $a_{\alpha,p}$. Finally, the application of formula (6.1) requires the computation of a volume integral.

Formula (6.3) yields exact evaluation of the moment of the coefficient against the test function. It has the following advantages over (6.1): the continuity of the coefficients is no longer necessary; the basic function $K^m[\alpha, p; b]$ is easier to determine (one-dimensional problems on $(0, \omega)$) and less singular than $\Psi_{z_0}^{3D}$. But it is still necessary to solve as many three-dimensional problems (6.4) as values of test functions b .

Formula (6.5) is closer to the idea of the quasi-dual formulas, since it is no longer necessary to solve three-dimensional problems for the determination of the dual functionals, but it does require the knowledge of the solution u . Still (6.5) is a volume integral, and the determination of the cut-off terms $\chi \overline{K}^m[\alpha, p; b]$ and $L(\chi \overline{K}^m[\alpha, p; b])$ is not obvious.

The quasi-dual formulas (4.9) and (5.2) need the determination of the same basic functions $K^m[\alpha, p; b]$ and the computation of the solution u itself, but no other three-dimensional solution. It requires only one (or a few) surface integrals, away from the edge where the functions $K^m[\alpha, p; b]$ are the most singular. Each determination of

$J[R](u, K^m[\beta, p; b])$ does not provide the exact value of the moment of $a_{\alpha, p}$ against b but its value modulo a (known) power of R , which allows a Richardson extrapolation of the limit from the computation of $J[R](u, K^m[\beta, p; b])$ for 3 values of R .

The works [34] in two dimensions and [36] in three dimensions also introduce an extraction method based on integration over a circular arc of radius R , followed by Richardson extrapolation in R . They are successfully implemented in an engineering stress analysis code. In a certain sense, they are precursory to our present method, with the following important distinction: In these two references the antisymmetric duality pairing $J[R]$ is replaced by a simple scalar product involving only the angular part of the singular functions. This possibility exists only for the Laplace operator due to its natural separation of variables (see [36]) and for the Lamé equations in two dimensions (see [34]). In order to reach a wide generality, we are led to deal with the universal duality pairing $J[R]$. On the other hand, the extraction done in [36] yields *pointwise* values of the coefficients. Extracting *moments* is more suitable to the regularity properties of the edge coefficients near corners and to the approximation by finite elements.

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