

A Method to Compute the Surface Green's Function of a Piezoelectric Half-Space

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ABSTRACT. The Piezoelectric Surface Acoustic Wave devices (so called SAW Components) are currently used today for frequency filtering, their main applications being to digital telecommunication systems. The need to improve their designs requires the development of accurate mathematical models to predict their physical performance. We develop here one of the essential tools used in these simulations : the 3D Green's function.

1. Introduction

This work is devoted to the computation of the 3D Green's function associated with Piezoelectric Surface Acoustic Wave Components. Our purpose is to generalize the techniques used to obtain the 2D Green's function (see [9]), to design a technique for the three dimensional case.

This paper is organized as follows: First we formulate the model problem (treated extensively in several articles and Ph.D theses, for example see [2], [3], [4], [6], [8], [9] and [11]). Next, we describe the methodological steps to obtain the 3D Spectral Green's Function. Finally, we compute the 3D Spatial Green's Function by an inverse Fourier transform : we analyze each singular contribution analytically and we propose a numerical method based on an FFT technique for the treatment of the regular part.

2. Setting the Mathematical Model

We consider a piezoelectric material filling the whole upper half-space $\mathbb{R}_+^3 := \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 / x_2 > 0\}$. The lower half-space $\mathbb{R}_-^3 := \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 / x_2 < 0\}$ represents a vacuum domain and we denote by $\Gamma := \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 / x_2 = 0\}$ the common boundary between both media. The unit normal vector on the boundary Γ is considered pointing to the interior of \mathbb{R}_+^3 , that is $\mathbf{n} = (0, 1, 0)$. The vacuum is only described by the permittivity of free space ($\epsilon_0 \in \mathbb{R}$).

In general, the piezoelectric materials are described by complex tensors. However, we assume here that the coefficients of those tensors are real constants and we denote them by :

- C_{ijkl} : the coefficients of the elasticity tensor for a constant electric field,
- e_{kij} : the coefficients of the piezoelectric tensor,
- ϵ_{ik} : the coefficients of the permittivity tensor for a constant deformation,
- ρ : the density of the piezoelectric material.

These coefficients have the following symmetry properties (see [1]) : $C_{ijkl} = C_{klij} = C_{ijlk} = C_{jilk}$, $e_{ikl} = e_{ilk}$ and $\epsilon_{ik} = \epsilon_{ki}$.

We adopt the following advantageous matrix and vector notations :

$$(2.1) \quad C_{jl} = \begin{pmatrix} C_{1j1l} & C_{1j2l} & C_{1j3l} \\ C_{2j1l} & C_{2j2l} & C_{2j3l} \\ C_{3j1l} & C_{3j2l} & C_{3j3l} \end{pmatrix}, \quad \mathbf{e}_{jl} = \begin{pmatrix} e_{j1l} \\ e_{j2l} \\ e_{j3l} \end{pmatrix}, \quad A_{jl} = \begin{pmatrix} C_{jl} & \mathbf{e}_{lj} \\ \mathbf{e}_{jl}^t & -\epsilon_{jl} \end{pmatrix} \quad 1 \leq j, l \leq 3.$$

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For all regular vector-valued function $\mathbf{v} = (v_1, v_2, v_3, v_4) : \mathbb{R}_+^3 \rightarrow^4$ for which derivatives make sense, we define the tensor field $T(\mathbf{v}) = (T_{ij}(\mathbf{v}))$ by :

$$(2.2) \quad T_{ij}(\mathbf{v}) = \sum_{k=1}^3 \left[\left(\sum_{l=1}^3 C_{ijkl} \frac{\partial v_l}{\partial x_k} \right) + e_{kij} \frac{\partial v_4}{\partial x_k} \right] \quad 1 \leq i, j \leq 3.$$

Analogously, we define the vector $\mathbf{D}(\mathbf{v}) = (D_i(\mathbf{v}))$ by the expression :

$$(2.3) \quad D_i(\mathbf{v}) = \sum_{k=1}^3 \left[\left(\sum_{l=1}^3 e_{jkl} \frac{\partial v_l}{\partial x_k} \right) - \epsilon_{jk} \frac{\partial v_4}{\partial x_k} \right] \quad 1 \leq i \leq 3.$$

3. The surface Green's function

For a given frequency $\omega > 0$, the surface Green's function is the impulse response of a media to an electric or stress excitation applied over its surface. It is defined by a 4×4 matrix linking the normal stress and the surface density of charge (the sources), with the mechanical stress and the electric potential (the waves). This relation is established by the convolution :

$$(3.1) \quad \begin{pmatrix} \mathbf{u}_p(\mathbf{x}) \\ \phi(\mathbf{x}) \end{pmatrix} = \int_{\Gamma} \mathbf{G}_{\mathbf{y}}(\omega, \mathbf{x}) \begin{pmatrix} \mathbf{T}(\mathbf{u}_p, \phi) \mathbf{n} \\ (\mathbf{D}(\mathbf{u}_p, \phi) +_0 \nabla \phi) \cdot \mathbf{n} \end{pmatrix}(\mathbf{y}) dS(\mathbf{y}), \quad \forall \mathbf{x} \in \Gamma.$$

The surface Green's function $\mathbf{G}_{\mathbf{y}}(\omega, \mathbf{x})$ is computed taking a source point $\mathbf{y} = (y_1, 0, y_3) \in \Gamma$. Since there is no horizontal variation in the geometry of the problem, we can suppose for the moment that $y_1 = y_3 = 0$. Denote by \mathbf{g}_q ($q = 1, \dots, 4$) the q^{th} column vector of the matrix $\mathbf{G}_{\mathbf{y}} = (g_{lq})$. In order to have the integral representation (3.1), our surface Green's function must be solution (in a distribution sense) of the coupled systems :

$$(P_+) \left\{ \begin{array}{ll} -\operatorname{div} \mathbf{T}(\mathbf{g}_q) - \rho \omega^2 \begin{pmatrix} g_{1q} \\ g_{2q} \\ g_{3q} \end{pmatrix} = \mathbf{0} & \text{in } \mathbb{R}_+^3, \quad 1 \leq q \leq 4 \\ -\operatorname{div} \mathbf{D}(\mathbf{g}_q) = 0 & \text{in } \mathbb{R}_+^3, \quad 1 \leq q \leq 4 \\ \mathbf{T}(\mathbf{g}_q) \mathbf{n} = \delta(x_1, x_3) \begin{pmatrix} \delta_{1q} \\ \delta_{2q} \\ \delta_{3q} \end{pmatrix} & \text{on } \Gamma, \quad 1 \leq q \leq 4 \\ (\mathbf{D}(\mathbf{g}_q) +_0 \nabla g_{4q}) \cdot \mathbf{n} = \delta(x_1, x_3) \delta_{4q} & \text{on } \Gamma, \quad 1 \leq q \leq 4 \\ + \text{Radiation Condition} & \text{when } |x| \rightarrow \infty. \end{array} \right.$$

$$(P_-) \left\{ \begin{array}{ll} -\Delta g_{4q} = 0 & \text{in } \mathbb{R}_-^3, \quad 1 \leq q \leq 4 \\ [g_{4q}] = 0 & \text{on } \Gamma, \quad 1 \leq q \leq 4 \\ + \text{Radiation Condition} & \text{when } |x| \rightarrow \infty. \end{array} \right.$$

Notice that the symbol $\delta(x_1, x_3)$ denotes the Dirac's delta in \mathbb{R}^2 while δ_{lq} denotes the usual Kronecker's delta. The brackets $[\cdot]$ represents the jump of the function over the surface.

3.1. Modes analysis.

3.1.1. *Vacuum modes.* Taking a Fourier transform in the directions x_1 and x_3 , the problem (P_-) becomes :

$$(3.2) \quad \begin{cases} -\frac{\partial^2 \widehat{g}_{4q}}{\partial x_2^2} + (k_1^2 + k_3^2) \widehat{g}_{4q} = 0 & \{x_2 < 0\}, \\ \widehat{g}_{4q} = \widehat{g}_{4q}(0) & \{x_2 = 0\}, \\ \widehat{g}_{4q} \text{ has to be bounded when } x_2 \rightarrow -\infty. \end{cases}$$

For $1 \leq q \leq 4$, the bounded solutions of equation (3.2) are :

$$(3.3) \quad \widehat{g}_{4q}(k_1, x_2, k_3) = \widehat{g}_{4q}(k_1, 0, k_3) e^{x_2 \sqrt{k_1^2 + k_3^2}}, \quad 1 \leq q \leq 4.$$

3.1.2. *Piezoelectric modes.* After a Fourier transform in the directions x_1 and x_3 , (P_+) becomes the initial value problem :

$$(3.4) \quad \begin{cases} -A_{22} \frac{d^2 \widehat{\mathbf{g}}_q}{dx_2^2} + i(k_1(A_{21} + A_{12}) + k_3(A_{23} + A_{32})) \frac{d\widehat{\mathbf{g}}_q}{dx_2} + \\ + (k_1^2 A_{11} + k_1 k_3 (A_{13} + A_{31}) + k_3^2 A_{33} - \rho \omega^2 A_{00}) \widehat{\mathbf{g}}_q = \mathbf{0} & \{x_2 > 0\}, \\ A_{22} \frac{d\widehat{\mathbf{g}}_q}{dx_2} - i(k_1 A_{21} + k_3 A_{23}) \widehat{\mathbf{g}}_q + 0 \frac{\partial \widehat{g}_{q4}}{\partial x_2}(k_1, 0, k_3) \mathbf{e}_4 = \frac{\mathbf{e}_q}{2\pi} & \{x_2 = 0\}, \\ \widehat{\mathbf{g}}_q \text{ satisfies a admissible mode condition.} \end{cases}$$

The matrices A_{jl} are defined in (2.1) and $A_{00} := \text{diag}\{1, 1, 1, 0\}$. The vector \mathbf{e}_q is the q^{th} vector in the canonical basis of \mathbb{R}^4 (\mathbf{e}_4 is the 4th one).

We define the following vectors :

$$(3.5) \quad \widehat{\mathbf{t}}_q := iA_{22} \frac{d\widehat{\mathbf{g}}_q}{dx_2} + (k_1 A_{21} + k_3 A_{23}) \widehat{\mathbf{g}}_q \quad \text{and} \quad \mathbf{w}_q = \begin{pmatrix} \widehat{\mathbf{g}}_q \\ \widehat{\mathbf{t}}_q \end{pmatrix}.$$

From now on, we will work with the normalized variables $s_1 = \frac{k_1}{\omega}$ and $s_3 = \frac{k_3}{\omega}$.

When $x_2 > 0$, a simple computation shows that \mathbf{w}_q satisfies the first order ordinary differential equation :

$$(3.6) \quad \frac{i}{\omega} \frac{d\mathbf{w}_q}{dx_2} = B \mathbf{w}_q, \quad \{x_2 > 0\},$$

where B is the 8×8 matrix whose entries in terms of 4×4 matrices are :

$$(3.7) \quad \begin{cases} B_{11} = -A_{22}^{-1} (s_1 A_{21} + s_3 A_{23}) \\ B_{12} = \omega^{-1} A_{22}^{-1} \\ B_{21} = \omega (s_1 A_{12} + s_3 A_{32}) A_{22}^{-1} (s_1 A_{21} + s_3 A_{23}) \\ \quad - \omega (s_1^2 A_{11} + s_1 s_3 (A_{13} + A_{31}) + s_3^2 A_{33} - \rho A_{00}) \\ B_{22} = -(s_1 A_{12} + s_3 A_{32}) A_{22}^{-1}. \end{cases}$$

For the applications, the matrix A_{22} (which only depends on the characteristics of the piezoelectric material) is a non singular matrix.

We want to study the independent solutions (modes) of equation (3.6). We start the analysis looking at the spectral problem for the matrix B . So we look for the values λ such that there exists a non zero vector :

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \text{ satisfying } (B - \lambda I) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \mathbf{0}.$$

From the equation above, we observe that the vector \mathbf{v} can be easily computed in terms of \mathbf{u} as :

$$(3.8) \quad \mathbf{v} = \omega (\lambda A_{22} + s_1 A_{21} + s_3 A_{23}) \mathbf{u}.$$

Then, the eigenproblem is reduced to find the nontrivial solutions of :

$$(3.9) \quad A(s_1, \lambda, s_3) \mathbf{u} = \mathbf{0},$$

where,

$$(3.10) \quad A(s_1, \lambda, s_3) = \lambda^2 A_{22} + \lambda s_1 (A_{21} + A_{12}) + \lambda s_3 (A_{23} + A_{32}) + s_1^2 A_{11} + s_1 s_3 (A_{13} + A_{31}) + s_3^2 A_{33} - \rho A_{00}.$$

Thus, for fixed s_1 and s_3 , the eigenvalues can be computed as the roots of the eight degree polynomial in λ :

$$(3.11) \quad \det(A(s_1, \lambda, s_3)) = 0.$$

It is not difficult to show that the equation (3.11) has eight different roots $\{\lambda_j\}_{j=1}^8$ for almost all $(s_1, s_3) \in \mathbb{R}^2$. Hence, the matrix $B = B(s_1, s_3)$ is diagonalizable a.e. in \mathbb{R}^2 . If the spectral pair $(\lambda_j, \mathbf{u}_j)$ is a solution of equation (3.9), then the set :

$$(3.12) \quad \{\mathbf{u}_j e^{-i\omega \lambda_j x_2}\}_{j=1}^8$$

is a set of independent solutions of the differential equation of problem (3.4). Moreover, the initial conditions of these solutions are respectively in the set :

$$(3.13) \quad \{-i\mathbf{v}_j\}_{j=1}^8,$$

where each \mathbf{v}_j is related with \mathbf{u}_j by the equation (3.8).

From the set (3.12) we consider as admissible modes, the ones associated with complex eigenvalues λ_j with $\Im m(\lambda_j) > 0$.

For real eigenvalues $\lambda_j \in \mathbb{R}$, the corresponding vectors \mathbf{u}_j and \mathbf{v}_j are real valued. The associated plane wave $\mathbf{u}_j e^{-i\omega(s_1 x_1 + \lambda_j x_2 + s_3 x_3)}$ is interpreted as a propagative electroelastic wave in the volume. The transported energy of such a wave is given by the Poynting vector $\mathcal{P} = (\mathcal{P}_i)$ (see [3] or [9]), which in this case has the expression :

$$(3.14) \quad \mathcal{P}_i = \frac{\omega^2}{2} \mathbf{u}_j^t (s_1 A_{i1} + \lambda_j A_{i2} + s_3 A_{i3}) \mathbf{u}_j.$$

Since there is no acoustic source into the piezoelectric material, the waves must not transport the energy towards the surface. Hence we look for plane waves satisfying $\mathcal{P}_2 > 0$. In conclusion, when $\lambda_j \in \mathbb{R}$, the solution $\mathbf{u}_j e^{-i\omega \lambda_j x_2}$ will be admissible if it satisfies the condition :

$$(3.15) \quad \mathbf{u}_j \cdot \mathbf{v}_j > 0.$$

It can be shown (for almost all $(s_1, s_3) \in \mathbb{R}^2$) that there are always four and only four admissible modes.

3.2. The spectral Green's function. Let U be the 4×4 matrix such that the column vectors are composed by the admissible $\{\mathbf{u}_j\}_{j=1, \dots, 4}$. Each $\hat{\mathbf{g}}_q$ must be written as a linear combination of the $\{\mathbf{u}_j e^{-i\omega \lambda_j x_2}\}_{j=1, \dots, 4}$. So when $x_2 = 0$, the spectral surface Green function should have an expression of the form :

$$(3.16) \quad \hat{\mathbf{G}} \Big|_{x_2=0} = U H,$$

for a matrix H containing the coefficients of the linear combinations.

Let V be the matrix whose column vectors are composed by the set $\{\omega^{-1} \mathbf{v}_j\}_{j=1, \dots, 4}$, where each \mathbf{v}_j is related with the admissible mode $\mathbf{u}_j e^{-i\omega \lambda_j x_2}$ by formula (3.8). The matrices U and V are independent from frequency, so we can compute them without knowing the value of $\omega > 0$. The computation of matrix V is straightforward from U :

$$(3.17) \quad \begin{cases} V &= A_{22} U \text{diag}\{\lambda_1, \dots, \lambda_4\} + (s_1 A_{12} + s_3 A_{32}) U \\ &= (A_{22} U \text{diag}\{\lambda_1, \dots, \lambda_4\} U^{-1} + s_1 A_{12} + s_3 A_{32}) U. \end{cases}$$

Let I the identity matrix and I_4 be the 4×4 matrix having the value 1 in the intersection of the 4th column with the 4th row and zero in all the others entries. By the initial conditions of the system (3.4), we get :

$$(3.18) \quad -i\omega V H + \omega \sqrt{s_1^2 + s_3^2} I_4 U H = \frac{1}{2\pi} I.$$

So the unknown matrix H has the form :

$$(3.19) \quad H = \frac{1}{2\pi\omega} \left(-iV +_0 \sqrt{s_1^2 + s_3^2} I_4 U \right)^{-1},$$

provided that the matrix on the left-hand side is invertible. Finally, from equation (3.16) we get the expression for the spectral surface Green function :

$$(3.20) \quad \widehat{\mathbf{G}} \Big|_{x_2=0} = \frac{1}{2\pi\omega} U \left(-iV +_0 \sqrt{s_1^2 + s_3^2} I_4 U \right)^{-1}.$$

An easy way to compute the matrix on the left-hand side of equation (3.20), can be done introducing the ω -independent matrix :

$$(3.21) \quad W = (W_{ql}) = U V^{-1} = (A_{22} U \text{diag}\{\lambda_1, \dots, \lambda_4\} U^{-1} + s_1 A_{12} + s_3 A_{32})^{-1}.$$

If $W_{44} \neq i_0^{-1}(s_1^2 + s_3^2)^{-\frac{1}{2}}$, matrix W allows to write equation (3.20) as :

$$(3.22) \quad \widehat{\mathbf{G}} \Big|_{x_2=0} = \frac{i}{2\pi\omega} W \left(I + i_0 \sqrt{s_1^2 + s_3^2} I_4 W \right)^{-1}.$$

So each component of $-2\pi i\omega \widehat{\mathbf{G}} \Big|_{x_2=0}$ can be computed independently from frequency $\omega > 0$ by :

$$(3.23) \quad -2\pi i\omega \hat{g}_{lq} = W_{lq} - i\epsilon_0 \sqrt{s_1^2 + s_3^2} \frac{W_{l4} W_{4q}}{1 + i\epsilon_0 \sqrt{s_1^2 + s_3^2} W_{44}}, \quad l = 1\dots 4, \quad q = 1\dots 4.$$

3.3. The spatial Green's function. We obtain the spatial surface Green's function as the double inverse Fourier transform of the spectral surface Green's function. Having equation (3.23) in mind we write :

$$(3.24) \quad \begin{aligned} \mathbf{G}_0(\omega, x_1, x_3) &= \frac{i}{(2\pi)^2 \omega} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} -2\pi i\omega \widehat{\mathbf{G}} \Big|_{x_2=0} e^{-i(k_1 x_1 + k_3 x_3)} dk_1 dk_3 \\ &= \frac{i\omega}{(2\pi)^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} -2\pi i\omega \widehat{\mathbf{G}} \Big|_{x_2=0} e^{-i\omega(s_1 x_1 + s_3 x_3)} ds_1 ds_3. \end{aligned}$$

So when the source point $\mathbf{y} = (y_1, 0, y_3)$ is not necessarily the origin, the surface Green's function has the expression :

$$(3.25) \quad \mathbf{G}_y(\omega, x_1, x_3) = \frac{i\omega}{(2\pi)^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} -2\pi i\omega \widehat{\mathbf{G}} \Big|_{x_2=0} e^{-i\omega(s_1(x_1 - y_1) + s_3(x_3 - y_3))} ds_1 ds_3.$$

An interesting approach to reduce one of the Fourier transforms, is to work with some special kind of polar coordinates :

$$(3.26) \quad \bar{s} = \begin{cases} \sqrt{s_1^2 + s_3^2} & \text{if } s_3 > 0 \\ s_3 & \text{if } s_3 = 0 \\ -\sqrt{s_1^2 + s_3^2} & \text{if } s_3 < 0 \end{cases} \quad \text{and} \quad \bar{\Phi} = \text{arctg} \left(\frac{s_3}{s_1} \right).$$

Thus, the (s_1, s_3) -plane is described by $\bar{s} \in]-\infty, +\infty[$ and $\bar{\Phi} \in [0, \pi[$.

In that way equation (3.25) reduces to :

$$(3.27) \quad \mathbf{G}_y(\omega, x_1, x_3) = \frac{i\omega}{(2\pi)^2} \int_0^\pi \int_{-\infty}^{+\infty} -2\pi i\omega \sqrt{\bar{s}^2} \widehat{\mathbf{G}} \Big|_{x_2=0} e^{-i\bar{s}\omega((x_1 - y_1) \sin \bar{\Phi} + (x_3 - y_3) \cos \bar{\Phi})} d\bar{s} d\bar{\Phi}.$$

We can define the following spectral function (independent from frequency $\omega > 0$) :

$$(3.28) \quad \widehat{F}_{\bar{\Phi}}(\bar{s}) := -2\pi i\omega \sqrt{\bar{s}^2} \widehat{\mathbf{G}} \Big|_{x_2=0}.$$

Plugging this definition into equation (3.27) we see that the second integral can be looked (formally) as a Fourier transform :

$$(3.29) \quad \left\{ \begin{array}{l} \mathbf{G}_{\mathbf{y}}(\omega, x_1, x_3) = \frac{i\omega}{(2\pi)^2} \int_0^\pi \int_{-\infty}^{+\infty} \widehat{F}_{\bar{\Phi}}(\bar{s}) e^{-i\bar{s}\omega((x_1-y_1)\sin\bar{\Phi}+(x_3-y_3)\cos\bar{\Phi})} d\bar{s} d\bar{\Phi} \\ = \frac{i\omega}{2\pi} \int_0^\pi F_{\bar{\Phi}}[\omega((x_1-y_1)\sin\bar{\Phi}+(x_3-y_3)\cos\bar{\Phi})] d\bar{\Phi}. \end{array} \right.$$

4. The numerical computation

The numerical application of the Fourier transform is very unstable, due to singularities and slow decay at infinity of the spectral surface Green's function $\hat{\mathbf{G}}$ (see [3] or [9]). To avoid this difficulty, we isolate these bad behaviors and we treat them analytically. Only the remaining regular part will be treated numerically by an FFT (Fast Fourier Transform) technique. Thus, we split $\hat{\mathbf{G}}$ in such a way that $\hat{\mathbf{G}} = \hat{\mathbf{G}}_{\text{regular}} + \hat{\mathbf{G}}_{\text{singular}}$.

4.1. Treatment of the singular part. We analyze in this section the singularities due to the existence of poles, the singularity in a neighbourhood of zero ($\bar{s} = 0$) and the slow decay at infinity.

4.1.1. *Treatment of the poles.* In [6] we describe a technique to compute the poles of $\hat{\mathbf{G}}$, which in fact, it is a curve of singularities. We know that the expression for this singular part, in polar coordinates \bar{s} and $\bar{\Phi}$, is given by :

$$(4.1) \quad \hat{\mathbf{G}}^{pole}(\bar{s}, \bar{\Phi}) = \frac{Q(\bar{s}_p(\bar{\Phi}), \bar{\Phi})(\bar{s} + \bar{s}_p(\bar{\Phi}))}{(\bar{s}^2 - \bar{s}_p^2(\bar{\Phi}))} + \frac{Q(-\bar{s}_p(\bar{\Phi}), \bar{\Phi})(\bar{s} - \bar{s}_p(\bar{\Phi}))}{(\bar{s}^2 - \bar{s}_p^2(\bar{\Phi}))},$$

where $\bar{s}_p(\bar{\Phi})$ is the parametrization of the curve of singularities and $Q(\bar{s}_p(\bar{\Phi}), \bar{\Phi})$ is an associated regular (4×4) matrix (see [6] for the details). Using the inverse Fourier transform (equation (3.27)), we get :

$$(4.2) \quad \mathbf{G}_{\mathbf{y}}^{pole}(\omega, x_1, x_3) = \frac{i\omega}{4\pi^2} \int_0^\pi \int_{-\infty}^{+\infty} \left[\frac{Q(\bar{s}_p(\bar{\Phi}), \bar{\Phi})(\bar{s} + \bar{s}_p(\bar{\Phi}))}{(\bar{s}^2 - \bar{s}_p^2(\bar{\Phi}))} + \frac{Q(-\bar{s}_p(\bar{\Phi}), \bar{\Phi})(\bar{s} - \bar{s}_p(\bar{\Phi}))}{(\bar{s}^2 - \bar{s}_p^2(\bar{\Phi}))} \right] \sqrt{\bar{s}^2} e^{-i\bar{s}u} d\bar{s} d\bar{\Phi},$$

where $u = \omega((x_1 - y_1)\cos\bar{\Phi} + (x_3 - y_3)\sin\bar{\Phi})$.

We like to compute an exact expression for the following quantities :

$$(4.3) \quad \left\{ \begin{array}{l} F_{\bar{\Phi}}^1(u) = \int_{-\infty}^{+\infty} \frac{\sqrt{\bar{s}^2}(\bar{s} + \bar{s}_p(\bar{\Phi}))e^{-i\bar{s}u}}{(\bar{s}^2 - \bar{s}_p^2(\bar{\Phi}))} d\bar{s} \\ \text{and} \\ F_{\bar{\Phi}}^2(u) = \int_{-\infty}^{+\infty} \frac{\sqrt{\bar{s}^2}(\bar{s} - \bar{s}_p(\bar{\Phi}))e^{-i\bar{s}u}}{(\bar{s}^2 - \bar{s}_p^2(\bar{\Phi}))} d\bar{s}. \end{array} \right.$$

With the help of the residue theorem [10] we can obtain an expression for the integrals in (4.3). Then, it can be shown that (see [7]) :

$$(4.4) \quad \mathbf{G}_{\mathbf{y}}^{pole}(\omega, x_1, x_3) = -\frac{\omega}{2\pi} \int_0^\pi Q(\text{sign}(u)\bar{s}_p(\bar{\Phi}), \bar{\Phi}) \sqrt{\bar{s}_p^2(\bar{\Phi})} \text{sgn}(u) e^{-i\bar{s}_p(\bar{\Phi})|u|} d\bar{\Phi}.$$

4.1.2. *Singularity in a neighbourhood of zero ($\bar{s} = 0$).* Due to the electrostatic behavior of the equation, the surface spectral Green's function presents on the 4,4 component, a singularity of the form :

$$(4.5) \quad \hat{g}_{44}^Z(\bar{s}, \bar{\Phi}) = \frac{C(\bar{\Phi})}{\omega \sqrt{\bar{s}_1^2 + \bar{s}_3^2}},$$

where $C(\bar{\Phi})$ is a complex function of the variable $\bar{\Phi}$.

We can prove (see [7] for the details) that the equation (4.5) is the Fourier transform of :

$$(4.6) \quad g_{44}^Z(x_1, x_3, y_1, y_3) = \frac{C'(\tan^{-1}(\frac{x_3 - y_3}{x_1 - y_1}))}{\sqrt{(x_1 - y_1)^2 + (x_3 - y_3)^2}},$$

where $C'(\cdot)$ is a function related to $C(\bar{\Phi})$.

4.1.3. *Treatment of the behavior at infinity.* The Spectral Green's function presents a behavior at infinity given by the Fourier transform of the fundamental solution of the static problem, which correspond to problems (P_+) and (P_-) when $\omega = 0$.

It is possible to prove using some properties of the matrices A_{jl} , that when $\omega = 0$, the 3D spatial Green's function on the surface may be written as :

$$(4.7) \quad \mathbf{G}^\infty(x_1, x_3, y_1, y_3) = \frac{C_0}{\sqrt{(x_1 - y_1)^2 + (x_3 - y_3)^2}} + \frac{C_1 \left(\tan^{-1} \left(\frac{x_3 - y_3}{x_1 - y_1} \right) \right)}{\sqrt{(x_1 - y_1)^2 + (x_3 - y_3)^2}},$$

for some complex constant C_0 and a function C_1 depending on the angle (see [7] for the details).

4.2. Treatment of the regular part. Once the singularities are isolated as much as possible, we use a numerical technique to treat the regular part of $\hat{\mathbf{G}}$ ($\hat{\mathbf{G}}^{reg}$). We propose here to use equation (3.27), to obtain the Spatial Green's function of the regular part :

$$(4.8) \quad \mathbf{G}_{\mathbf{y}}^{reg}(\omega, x_1, x_3) = \frac{i\omega}{4\pi^2} \int_0^\pi \int_{-\infty}^{+\infty} \hat{\mathbf{G}}^{reg}(\bar{s}, \bar{\Phi}) \sqrt{\bar{s}^2} e^{-i\omega\bar{s}((x_1 - y_1) \cos \bar{\Phi} + (x_3 - y_3) \sin \bar{\Phi})} d\bar{s} d\bar{\Phi}$$

The first integral on $(]-\infty, +\infty[)$ is treated numerically using an FFT technique :

$$(4.9) \quad \mathbf{F}_{\bar{\Phi}}^{reg}(u) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{\mathbf{F}}_{\bar{\Phi}}^{reg}(\bar{s}) e^{-i\bar{s}u} d\bar{s} \approx FFT \left(\hat{\mathbf{F}}_{\bar{\Phi}}^{reg}(\bar{s}) \right)$$

where $u = \omega((x_1 - y_1) \cos \bar{\Phi} + (x_3 - y_3) \sin \bar{\Phi})$ and $\hat{\mathbf{F}}_{\bar{\Phi}}^{reg} = -2\pi i\omega \sqrt{\bar{s}^2} \hat{\mathbf{G}}^{reg}$ (which is independent from frequency $\omega > 0$).

In order to discretize the equation (4.9), we take a positive value $\bar{s}_{max} > 0$. Next we define the step $\Delta\bar{s} = \frac{2\bar{s}_{max}}{N}$ and the nodes $\bar{s}_n = -\bar{s}_{max} + n\Delta\bar{s}$, where $0 \leq n \leq N$, $N = 2^l$ and $l \in \mathbb{N}$.

For the u variable we take $u_{max} > 0$ and we define the step $\Delta u = \frac{2u_{max}}{N}$ and the nodes $u_m = -u_{max} + m\Delta u$, for $0 \leq m \leq N$.

By the Sampling Theorem, a band-limited signal can be reconstructed if the sampling frequency is greater than twice the bandwidth of the signal (otherwise aliasing would result). In other words we need to satisfy :

$$\Delta\bar{s} \Delta u = \frac{2\pi}{N} \quad \text{and} \quad 2\bar{s}_{max} u_{max} = \pi N.$$

Now, applying the trapezoidal rule to (4.9) we obtain :

$$(4.10) \quad \mathbf{F}_{\omega, \bar{\Phi}}^{reg}(u_m) \approx (-1)^m \frac{\Delta\bar{s}}{2\pi} \sum_{n=0}^{N-1} (-1)^n \hat{\mathbf{F}}_{\omega, \bar{\Phi}}^{reg}(\bar{s}_n) e^{-\frac{i2\pi mn}{N}} + (-1)^m \frac{\Delta\bar{s}}{4\pi} \left(\hat{\mathbf{F}}_{\omega, \bar{\Phi}}^{reg}(\bar{s}_N) - \hat{\mathbf{F}}_{\omega, \bar{\Phi}}^{reg}(\bar{s}_0) \right).$$

Finally, we discretize the variable $\bar{\Phi}$ by the nodes $\bar{\Phi}_j = j\pi/p$ ($j = 0, \dots, p-1$).

To have a good approximation for the $\bar{\Phi}$ -integral in (4.8) we need the condition (see [5]) :

$$p \geq 2\bar{s}_{max} u_{max}.$$

This method presents the advantage (with respect to a direct use of a double FFT) that we only need a great number of points in the computation of the radial integral over the interval $(]-\infty, +\infty[)$. The computation of the angle integral over $[0, \pi)$ uses only a few points.

5. Conclusions.

In this work, we have presented a method to obtain the 3D surface Green's function. First, we have seen how we may construct the spectral 3D Green's function employing the Fahmy-Adler Method's [2]. Afterwards, we obtain the 3D spatial Green function on the surface Γ as the Fourier transform of the spectral 3D Green's function. We analyse separately the singularities and the behavior at infinity from the regular part. We use semi-analytical techniques for the singularities and the behavior at infinity, and a FFT technique for the regular part.

Here, important changes with respect to the 2D case appears. We observe that is necessary to use numerical methods to compute the spatial contributions of the singularities and the behavior at infinity.

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