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Transformation of a heterogeneous acoustic wave equation into a Schrödinger equation to extend the scope of the localization landscape method

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Résumé — This abstract describes a transformation from a heterogeneous scalar (classical) wave equation to a Schrödinger equation with heterogeneous potential, which allows to extend the localization landscape technique to classical wave equations in 3D for a larger class of fluctuating parameters. That transformation is based on a coordinate mapping, dependent on the fluctuating velocity, and on a similarity transformation. The heterogeneous potential in the Schrödinger equation is an analytical function of the impedance of the acoustic equation. The use of this transformation to design a localization landscape technique for the acoustic wave equation is detailed.
Mots clés — Helmholtz equation ; Schrödinger equation ; Conformal mapping.

1 Introduction

This abstract describes a transformation from a heterogeneous Helmholtz equation to a Schrödinger equation with heterogeneous potential. Its objective is to help understand the precise similarities and differences between the classical wave equation and the Schrödinger equation. This transformation has already been used in 1D in various contexts. For instance in [4] under the name of point-canonical transformation, to transform a Schrödinger equation with position-dependent mass (akin to a heterogeneous Helmholtz equation) into a Schrödinger equation with position-independent mass (the "classical" Schrödinger equation). In [3], under the name of Liouville transformation, it helps to derive analytical solutions of Schrödinger equations in complex cases. Similarly, in 3D, it allows in [5] to derive analytical Green's functions for Helmholtz equation in heterogeneous media, to be used in the Boundary Element Method. In Section 2, we introduce a change of coordinates that will be useful for our transformation, and the impact this change has on the gradients appearing in Helmholtz equation. Section 3 describes the transformation from a Helmholtz equation with heterogeneous coefficients to a Schrödinger equation with heterogeneous potential, as well as the formula for that potential as a function of the coefficients of the Helmholtz equation. Finally, Section 4 discusses the extension of the localization landscape method from Schrödinger equation to classical wave equations. It is an extension of our previous paper [1], where the localization landscape method for acoustic waves was presented in 1D, and for density equal to compressibility, in which case the transformation introduced in Section 3 is not necessary.

2 Preliminary : change of coordinates in the Helmholtz equation

2.1 Setting

Consider a scalar potential ψ governed by the Helmholtz equation and homogeneous Dirichlet boundary conditions in a bounded medium $\Omega \subset \mathbb{R}^d$, with $1 \leq d \leq 3$, characterized by the position-dependent and bounded compressibility modulus $\kappa(\boldsymbol{x}) \geq \kappa_0 > 0$ and mass density $\rho(\boldsymbol{x}) \geq \rho_0 > 0$, i.e.

$$\begin{cases} \operatorname{div}\Big(\kappa(\boldsymbol{x})\boldsymbol{\nabla}\psi(\boldsymbol{x})\Big) = -\rho(\boldsymbol{x})\omega^2\psi(\boldsymbol{x}) & \forall \boldsymbol{x} \in \Omega \\ \psi(\boldsymbol{x}) = 0 & \forall \boldsymbol{x} \in \partial\Omega, \end{cases} \tag{1}$$

where ω is a circular frequency. To be used later on, we also introduce the position-dependent impedance $z(\boldsymbol{x})$ as

$$z(\boldsymbol{x}) = \sqrt{\kappa(\boldsymbol{x})\rho(\boldsymbol{x})}, \tag{2}$$

and c_0 a reference homogeneous wavespeed.

We consider an invertible *vector-valued* transformation $\boldsymbol{g}$, with inverse $\boldsymbol{F}$, which maps the coordinates $\boldsymbol{x} \in \Omega$ to $\boldsymbol{X} \in \Omega_g$, where Ω_g is a transformed domain, as

$$\boldsymbol{X} = \boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{F}^{-1}(\boldsymbol{x}), \tag{3}$$

and whose gradient is the second-order tensor $\boldsymbol{G} = \boldsymbol{\nabla}\boldsymbol{g}(\boldsymbol{x}) = \partial\boldsymbol{X}/\partial\boldsymbol{x}$, the Jacobian matrix of the transformation. In addition, we define $\boldsymbol{J} = \boldsymbol{G}^{-1}$, so that $\boldsymbol{J} = \partial\boldsymbol{x}/\partial\boldsymbol{X}$, and denote $\mathcal{J}(\boldsymbol{X}) = \det\boldsymbol{J}(\boldsymbol{X})$. Lastly, we use lowercase (resp. uppercase) letters hereafter to denote quantities expressed on Ω (resp. Ω_g), with

$$\psi(\boldsymbol{x}) = \psi(\boldsymbol{F}(\boldsymbol{X})) = \Psi(\boldsymbol{X}), \tag{4}$$

and likewise for K, P and Z relatively to κ, ρ and z, respectively.

2.2 Transformation laws

To transfer the problem (1) on the transformed domain Ω_g, we rewrite it in weak form as

$$\int_\Omega \kappa(\boldsymbol{x})\boldsymbol{\nabla}\psi(\boldsymbol{x})\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\mathrm{d}V_x = \int_\Omega \rho(\boldsymbol{x})\omega^2\psi(\boldsymbol{x})\phi(\boldsymbol{x})\mathrm{d}V_x \tag{5}$$

for all sufficiently smooth test function ϕ such that $\phi(\boldsymbol{x}) = 0$ on $\partial\Omega$.

We observe that

$$\boldsymbol{\nabla}\psi(\boldsymbol{x}) = \boldsymbol{J}^{-T}(\boldsymbol{X})\cdot\boldsymbol{\nabla}_X\Psi(\boldsymbol{X}) \tag{6}$$

with $\boldsymbol{\nabla}_X$ being the gradient operator relatively to the variable $\boldsymbol{X}$, and similarly for the divergence operator div_X to be used hereafter. Using that $\mathrm{d}V_x = \mathcal{J}(\boldsymbol{X})\mathrm{d}V_X$, operating a change of coordinates in (5), observing that, for any pair of matrices $\boldsymbol{A}$ and $\boldsymbol{B}$, $(\boldsymbol{J}^{-T}(\boldsymbol{X})\cdot\boldsymbol{A})\cdot(\boldsymbol{J}^{-T}(\boldsymbol{X})\cdot\boldsymbol{B}) = (\boldsymbol{J}^{-1}(\boldsymbol{X})\boldsymbol{J}^{-T}(\boldsymbol{X})\cdot\boldsymbol{A})\cdot\boldsymbol{B}$, and integrating by parts eventually yields that Ψ satisfies the following transformed wave equation in Ω_g :

$$\begin{cases} \mathrm{div}_X\Big(\boldsymbol{K}_g(\boldsymbol{X})\cdot\boldsymbol{\nabla}_X\Psi(\boldsymbol{X})\Big) = -P_g(\boldsymbol{X})\omega^2\Psi(\boldsymbol{X}) & \forall\boldsymbol{X}\in\Omega_g \\ \Psi(\boldsymbol{X}) = 0 & \forall\boldsymbol{X}\in\partial\Omega_g, \end{cases} \tag{7}$$

where the transformed compressibility modulus and mass density read

$$\boldsymbol{K}_g(\boldsymbol{X}) = \mathcal{J}(\boldsymbol{X})K(\boldsymbol{X})\boldsymbol{J}^{-1}(\boldsymbol{X})\cdot\boldsymbol{J}^{-T}(\boldsymbol{X}) \qquad \text{and} \qquad P_g(\boldsymbol{X}) = \mathcal{J}(\boldsymbol{X})P(\boldsymbol{X}). \tag{8}$$

We can notice that the obtained mass density P_g remains a scalar, while the compressibility $\boldsymbol{K}_g$ is potentially anisotropic, with symmetry $\boldsymbol{K}_g^T = \boldsymbol{K}_g$.

3 From (Hermann von) Helmholtz to (Erwin) Schrödinger equation

3.1 Mapping of the coordinates

3.1.1 Wavespeed-related metric

We now consider expanding the transformed Helmholtz equation (7) and using the symmetry of $\boldsymbol{K}_g$ to rewrite the former as

$$P_g^{-1}(\boldsymbol{X})\boldsymbol{K}_g(\boldsymbol{X}) : \boldsymbol{\nabla}_X\boldsymbol{\nabla}_X\Psi(\boldsymbol{X}) + P_g^{-1}(\boldsymbol{X})\big(\mathrm{div}_X\,\boldsymbol{K}_g(\boldsymbol{X})\big)\cdot\boldsymbol{\nabla}_X\Psi(\boldsymbol{X}) = -\omega^2\Psi(\boldsymbol{X}). \tag{9}$$

Following Peña, Morales et al., the objective is to find a mapping (3) such that

$$P_g^{-1}(\boldsymbol{X})\boldsymbol{K}_g(\boldsymbol{X}) : \boldsymbol{\nabla}_X\boldsymbol{\nabla}_X\Psi(\boldsymbol{X}) = c_0^2\Delta_X\Psi(\boldsymbol{X}),$$

where the reference wavespeed c_0 is introduced here for dimensional consistency. A sufficient condition for the above is

$$P_g^{-1}(\boldsymbol{X})\boldsymbol{K}_g(\boldsymbol{X}) = c_0^2\boldsymbol{I} \qquad \text{i.e.} \qquad \boldsymbol{J}^{-1}(\boldsymbol{X})\cdot\boldsymbol{J}^{-T}(\boldsymbol{X}) = \frac{P(\boldsymbol{X})}{K(\boldsymbol{X})}c_0^2\boldsymbol{I} \tag{10}$$

with $\boldsymbol{I}$ being the identity tensor. This condition implies that :

– the transformed medium is isotropic, as $\boldsymbol{K}_g(\boldsymbol{X}) = K_g(\boldsymbol{X})\boldsymbol{I}$ with K_g a scalar field,
– the wavespeed $C_g(\boldsymbol{X}) = \sqrt{K_g(\boldsymbol{X})/P_g(\boldsymbol{X})}$ is uniform and equal to c_0.

This amounts to redefine the space metric so as to transform the original non-uniform wavespeed field to a homogeneous one. Owing to (8) and the definition of the Jacobian, then (10) leads to the following equation for the gradient of the transformation :

$$\boldsymbol{G}(\boldsymbol{x})\cdot\boldsymbol{G}^T(\boldsymbol{x}) = \frac{\rho(\boldsymbol{x})}{\kappa(\boldsymbol{x})}c_0^2\boldsymbol{I}. \tag{11}$$

Eq. 11 is equivalent to stating that the transformation we are looking for is such that

$$\boldsymbol{G}(\boldsymbol{x}) = \boldsymbol{\nabla g}(\boldsymbol{x}) = c_0\sqrt{\frac{\rho(\boldsymbol{x})}{\kappa(\boldsymbol{x})}}\boldsymbol{R}. \tag{12}$$

where $\boldsymbol{R}$ is a rotation matrix, which in turn is equivalent to stating that

$$\frac{\partial g_x}{\partial \xi} = \frac{\partial g_y}{\partial \eta} = c_0\sqrt{\frac{\rho(\boldsymbol{x})}{\kappa(\boldsymbol{x})}}, \quad \frac{\partial g_x}{\partial \eta} = \frac{\partial g_y}{\partial \xi} = 0, \tag{13}$$

where (ξ,η) is the set of coordinates corresponding to (x,y) in the rotation $\boldsymbol{R}$. This corresponds to Cauchy-Riemann equations for the complex function $g_x + ig_y$. Hence, a transformation corresponding to $\rho(\boldsymbol{x})c_0^2/\kappa(\boldsymbol{x})$ can only be found if the latter function is the modulus squared of an analytic function. Through the maximum modulus principle, this in turn implies that $\rho(\boldsymbol{x})c_0^2/\kappa(\boldsymbol{x})$ cannot display local maxima.

3.2 Similarity transformation

Provided that the mapping $\boldsymbol{g}$ satisfies the condition obtained in the previous section then (10) implies that

$$P_g^{-1}(\boldsymbol{X})\big(\mathrm{div}_X\,\boldsymbol{K}_g(\boldsymbol{X})\big) = c_0^2P_g^{-1}(\boldsymbol{X})\boldsymbol{\nabla}_X P_g(\boldsymbol{X}) = c_0^2\boldsymbol{\nabla}_X\ln\big(P_g(\boldsymbol{X})\big).$$

Upon calculating the determinant of (10) we get that

$$\mathcal{J}(\boldsymbol{X}) = \frac{1}{c_0}\sqrt{\frac{K(\boldsymbol{X})}{P(\boldsymbol{X})}},$$

so that, according to (8), the gradient of $P_g(\boldsymbol{X})$ above can be recast into a following symmetric form in K, P as

$$\boldsymbol{\nabla}_X\ln\big(P_g(\boldsymbol{X})\big) = \boldsymbol{\nabla}_X\ln\left(\sqrt{K(\boldsymbol{X})P(\boldsymbol{X})}\right) = \boldsymbol{\nabla}_X\ln Z(\boldsymbol{X}) \tag{14}$$

in terms of the transformed impedance map $Z(\boldsymbol{X})$. Using these identities back in (9) leads to

$$\Delta_X\Psi(\boldsymbol{X}) + \frac{\boldsymbol{\nabla}_X Z(\boldsymbol{X})}{Z(\boldsymbol{X})}\cdot\boldsymbol{\nabla}_X\Psi(\boldsymbol{X}) = -\frac{\omega^2}{c_0^2}\Psi(\boldsymbol{X}). \tag{15}$$

Now, we define the field $\tilde{\Psi}(\boldsymbol{X})$ through the similarity transformation

$$\tilde{\Psi}(\boldsymbol{X}) = \Psi(\boldsymbol{X})\sqrt{Z(\boldsymbol{X})}, \tag{16}$$

which leads, after some calculs, to a Schrödinger equation for $\tilde{\Psi}$ that writes as

$$-\Delta_X\tilde{\Psi}(\boldsymbol{X}) + V_{\mathrm{eff}}(\boldsymbol{X})\tilde{\Psi}(\boldsymbol{X}) = \frac{\omega^2}{c_0^2}\tilde{\Psi}(\boldsymbol{X}), \tag{17}$$

where V_{eff} is a scalar effective potential defined locally as

$$V_{\mathrm{eff}}(\boldsymbol{X}) = \frac{1}{4}\left(2\frac{\Delta_X Z(\boldsymbol{X})}{Z(\boldsymbol{X})} - \frac{|\boldsymbol{\nabla}_X Z(\boldsymbol{X})|^2}{Z(\boldsymbol{X})^2}\right) = \Delta_X\ln\sqrt{Z(\boldsymbol{X})} + \left|\boldsymbol{\nabla}_X\ln\sqrt{Z(\boldsymbol{X})}\right|^2.$$

4 Localization landscape for 3D acoustic waves

Anderson localization is a universal interference phenomenon occurring when a wave evolves through a random medium and it has been observed in a great variety of physical systems, either quantum or classical. A recently developed localization landscape theory [2] offers a computationally affordable way to obtain useful information on the localized modes, such as their location or size. It was shown recently that this theory was not directly useful for acoustic waves, because the lowest eigenmodes (for largest $1/\omega_n^2$) are delocalized (opposite behavior from Schrödinger equation), and an extension was proposed in 1D [1] in the particular case $\rho = \kappa$. We propose here an extension in 3D and for $\rho(\boldsymbol{x}) \neq \kappa(\boldsymbol{x})$. In that case, the transformation presented in the previous chapter is necessary.

Starting from Eq. (1), which an eigenvalue problem, and hence numerically expensive, the localization landscape consists in rather solving the following boundary value problem, much cheaper numerically :

$$\begin{cases} \operatorname{div}\Big(\kappa(\boldsymbol{x})\boldsymbol{\nabla} u(\boldsymbol{x})\Big) = -\dfrac{\rho(\boldsymbol{x})}{\sqrt{z(\boldsymbol{x})}} & \forall \boldsymbol{x} \in \Omega \\ u(\boldsymbol{x}) = 0 & \forall \boldsymbol{x} \in \partial\Omega, \end{cases} \tag{18}$$

Of course, the result is less rich because we do not have the knowledge of the eigenfrequencies nor the eigenvectors. But the so-called landscape is expected to contain a lot of information on the support S_n of the different eigenmodes (labelled by $n \geq 0$) through the relation

$$S_n \approx \left\{ \boldsymbol{x} \in \Omega : u(\boldsymbol{x}) \geq \frac{1}{\omega_n^2} \right\}. \tag{19}$$

This relation has been proved only for Schrödinger so it is necessary to transform the acoustic wave equation (1) into Schrödinger, using the transformation of the previous section, in order to derive it. Although the results is correct, examples show that it does not bring useful insight for classical wave equations. Indeed, the lowest eigenmodes (for largest $1/\omega_n^2$) are delocalized, which in turn means that the landscape is way above all eigenmodes, bringing no insight into localized modes.

In line with our previous paper [1], interesting insight can be retrieved by considering a series of shifted problems, indexed by the frequency shift ω_s^2 :

$$\begin{cases} \operatorname{div}\Big(\kappa(\boldsymbol{x})\boldsymbol{\nabla} u(\boldsymbol{x},\omega_s^2)\Big) - \omega_s^2 \dfrac{\rho(\boldsymbol{x})}{\sqrt{z(\boldsymbol{x})}} u(\boldsymbol{x},\omega_s^2) = -\dfrac{\rho(\boldsymbol{x})}{\sqrt{z(\boldsymbol{x})}} & \forall \boldsymbol{x} \in \Omega \\ u(\boldsymbol{x}) = 0 & \forall \boldsymbol{x} \in \partial\Omega, \end{cases} \tag{20}$$

and defining a optimized localization landscape function in the original space

$$u^\star(\boldsymbol{x}) = \left(\max_{\omega_s^2} \left\{ \frac{1}{u(\boldsymbol{x};\omega_s^2)\sqrt{z(\boldsymbol{x})}} - \omega_s^2 \right\} \right)^{-1}. \tag{21}$$

Eventually, we retrieve the desired property Eq. (19), but with $u^\star(\boldsymbol{x})$ instead of $u(\boldsymbol{x})$. This is coherent with the formulas derived in [1] when $z(\boldsymbol{x}) = \rho(\boldsymbol{x}) = \kappa(\boldsymbol{x})$.

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