

# Plasmonic cavity modes: black-hole phenomena captured by Perfectly Matched Layers

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**Abstract**— We study a 2D dielectric cavity with a metal inclusion and we assume that, in a given frequency range, the metal permittivity  $\epsilon = \epsilon(\omega)$  is a negative real number. We look for the plasmonic cavity resonances by studying the linearized eigenvalue problem (dependence in  $\omega$  of  $\epsilon$  frozen). When the inclusion is smooth, the linearized problem operator has a discrete spectrum which can be computed numerically with a good approximation *e.g.* by a classical Finite Element Method. However, when the inclusion has corners, due to very singular phenomena, we loose the operator properties and numerical approximations are not stable. Paradoxically there is a theoretical and a numerical need to take into account these singularities in order to compute the modes, even the regular ones. Then we propose an original use of PMLs (Perfectly Matched Layers) at the corners to capture these plasmonic waves.

## 1. INTRODUCTION

Consider a cavity  $\Omega$  made of a dielectric material  $\Omega_1$  with a metal inclusion  $\Omega_2$ , which are separated by an interface  $\Sigma$ . We consider the time-harmonic Maxwell equations for the Transverse Magnetic

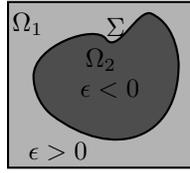


Figure 1: Example of a cavity with a smooth interface.

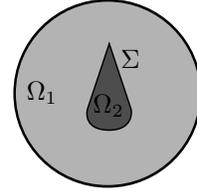


Figure 2: Example of a cavity where the interface has corners.

polarization. In the metal the permittivity  $\epsilon$  depends on the frequency  $\omega$  but for simplicity we study the *linearized* eigenvalue problem:

$$\left\{ \begin{array}{l} \text{Find } u \in H^1(\Omega), u \neq 0, \omega \in \mathbb{C} \text{ such that:} \\ -\operatorname{div} \left( \frac{1}{\epsilon} \nabla u \right) = \omega^2 \mu u \text{ in } \Omega \\ u = 0 \text{ on } \partial\Omega \end{array} \right. \Leftrightarrow \left\{ \begin{array}{l} \text{Find } u \in H_0^1(\Omega), u \neq 0, \omega \in \mathbb{C} \text{ such that:} \\ \int_{\Omega} \frac{1}{\epsilon} \nabla u \cdot \nabla \bar{v} \, d\Omega = \omega^2 \int_{\Omega} u \bar{v} \, d\Omega \quad \forall v \in H_0^1(\Omega) \end{array} \right. \quad (1)$$

where  $\mu$  denotes the magnetic permeability. We take  $\epsilon$  and  $\mu$  piecewise constant functions,  $\mu > 0$  almost everywhere and  $\epsilon$  sign changing through the interface  $\Sigma$ . Let's define the operator:

$$A : \left\{ \begin{array}{l} D(A) \subset L^2(\Omega) \longrightarrow L^2(\Omega) \\ u \longmapsto -\frac{1}{\mu} \operatorname{div} \left( \frac{1}{\epsilon} \nabla u \right) \end{array} \right. \text{ with } D(A) = \{u \in H_0^1(\Omega) / -\frac{1}{\mu} \operatorname{div} \left( \frac{1}{\epsilon} \nabla u \right) \in L^2(\Omega)\}.$$

Our goal is to find the eigenvalues of  $A$ . When  $\epsilon$  is not sign changing, one can easily prove that  $A$  is symmetric, self-adjoint and has a compact resolvent (called SC. properties in the rest of the paper). When  $\epsilon$  changes sign at the interface, these properties can still be satisfied under some conditions on  $\epsilon$  and the geometry of  $\Sigma$  [1]. These conditions lead to the existence of an isomorphism  $T$  of  $H_0^1(\Omega)$  such that the sesquilinear form is  $T$ -coercive :  $\int_{\Omega} \frac{1}{\epsilon} \nabla u \cdot \nabla \overline{Tu} \, d\Omega \geq \alpha \|u\|_{H_0^1(\Omega)}^2$  with  $\alpha > 0$ ,  $\alpha$  independent of  $u$ . Then the operator is self-adjoint and with compact resolvent. When these conditions are not satisfied, the operator  $A$  is no longer self-adjoint and neither has compact resolvent. Due to singular phenomena occurring at the corners, a new functional framework is required. In [2, 3] an

extension of the operator  $A$  is given which recovers the resolvent's compactness property. It takes into account singular functions whose gradient is not square integrable at the corners. Numerically, a specific treatment is required at the corners to capture these singularities. The first section is dedicated to solving the self-adjoint case, the next one to solving the non self-adjoint case, and the last one handles the non linear eigenvalue problem by taking into account the dependence in  $\omega$  of the permittivity.

## 2. THE SELF-ADJOINT CASE

When  $\epsilon$  changes sign, one can still have SC. properties for  $A$  if and only if [1] the ratio  $\kappa_\epsilon$  of permittivities between the dielectric and the metal (called the contrast) is such that:

- $\kappa_\epsilon \neq -1$  for a smooth interface  $\Sigma$  (see fig.1)
- $\kappa_\epsilon$  doesn't belong to a *critical interval*  $I_c$  containing  $\{-1\}$  when the interface  $\Sigma$  has corners (see fig.2)

$I_c$  is a function of the sharpest corner  $\theta$  ( $\theta < \pi$ ) given by  $I_c = [\frac{\theta-2\pi}{\theta}, \frac{\theta}{\theta-2\pi}]$ . Notice that when  $\theta \rightarrow \pi$ ,  $I_c \rightarrow \{-1\}$  and when  $\theta \rightarrow 0$ ,  $I_c \rightarrow \mathbb{R}^-$ . Having a sign changing permittivity yields the existence of both positive and negative eigenvalues. More precisely, the eigenvalues  $(\omega_i^2)_i$  have finite multiplicity and consist in two sequences of real numbers tending respectively to  $\pm\infty$  (see fig.7).

### Approximation of the eigenvalues outside the critical interval

In order to approximate the problem (1), we use standard conforming Lagrange Finite Elements of order 2. Under some conditions on the mesh [4], we can prove the convergence toward the exact eigenvalues without spurious modes [5]. We have made computations for the geometry of fig.2. We observe stability of the results with respect to the mesh size (see fig.3). The bigger in modulus the eigenvalue becomes, the more confined are the associated modes: in the metal for a negative eigenvalue, respectively in the dielectric for a positive one (see fig.4).

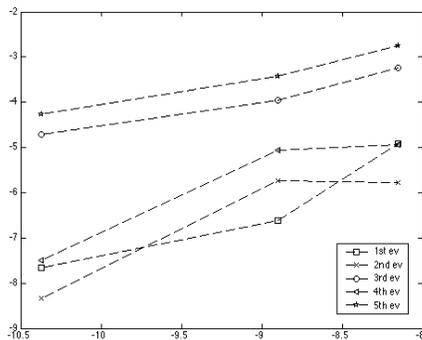


Figure 3: Approximation of the first eigenvalues  $\log(|\lambda_{\text{finer mesh}} - \lambda_{\text{coarser mesh}}|)$  for several mesh sizes. The numerical illustrations are realized with the following parameters: the metal's shape is a droplet with a sharp angle of  $\frac{\pi}{6}$ , and permittivities  $\epsilon_1 = 1$ ,  $\epsilon_2 = -13$ .

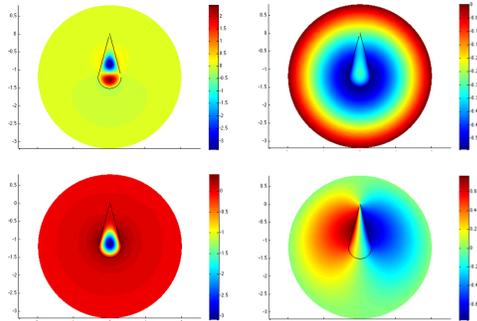


Figure 4: First modes of the SC operator, associated to the first eigenvalues (the smallest in modulus): the two on the left are associated to a negative eigenvalue, and the two on the right to a positive one. The numerical illustrations are realized on the finer mesh with the same parameters as fig.3.

## 3. THE NON SELF-ADJOINT CASE: AN ORIGINAL USE OF PMLS

For a contrast  $\kappa_\epsilon$  chosen in the critical interval (excluding  $-1$ ), since the problem (1) is ill-posed, there is no convergence of the Finite Element Method (see fig.5), and particular phenomena occur at the corner.

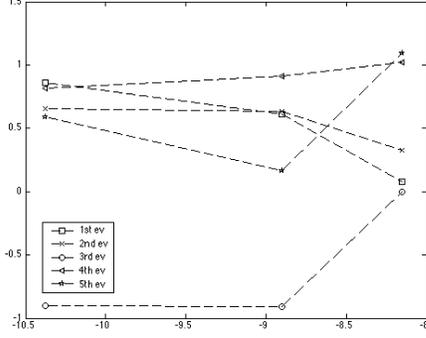


Figure 5: Approximation of the first eigenvalues  $\log(|\lambda_{\text{finer mesh}} - \lambda_{\text{coarser mesh}}|)$  for several mesh sizes inside the critical interval. The numerical illustrations are realized with a contrast  $\kappa_\epsilon = -\frac{1}{0.7} \in I_c$ .

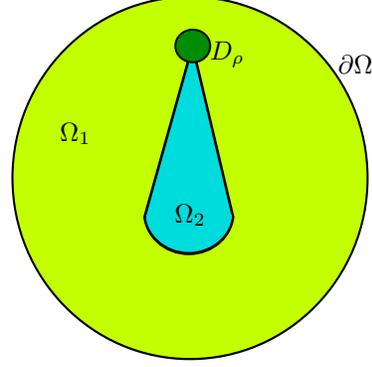


Figure 6: Scheme of the whole domain minus a small disk  $D_\rho$  at the corner.

Near the corner, an asymptotic analysis [2] let us know that, for  $\kappa_\epsilon$  in the critical interval, the magnetic field is a combination of separated variables functions plus a regular part:

$$u(r, \theta) \simeq u_{\text{cst}} + u_{\text{reg}} + c^+ s^+ + c^- s^-, \quad c^+, c^- \in \mathbb{C} \quad (2)$$

where  $u_{\text{cst}}$  is a constant number and  $s^\pm(r, \theta) = \phi(\theta)r^{\pm i\eta}$  ( $\eta \in \mathbb{R}$ ) can be interpreted as propagative waves propagating towards the corner, or from the corner:  $s^\pm$  are called black-hole waves. These singularities are responsible for the ill-posedness of the problem and their existence characterizes the critical interval. In [2, 3] extensions of the operator  $A$  are given that take into account the singularities  $s^\pm$ . We define an extension family  $A_\gamma$  of  $A$  such that  $D(A_\gamma) = D(A) \oplus \text{span}\{s_\gamma = s^+ + \gamma s^-\}$ . Then  $\forall u \in D(A_\gamma)$ ,  $u = u_A + \beta s_\gamma$ , with  $u_A \in D(A)$  and  $\beta \in \mathbb{C}$ . All extensions have compact resolvent, thus the extended operator spectrum will be discrete. If  $|\gamma| = 1$ ,  $A_\gamma$  is a self-adjoint extension according to [3]. Here we're going to choose a non self-adjoint extension in order to have an efficient numerical method. Let's motivate our choice by calculating the energy flux. In order to estimate the energy that goes towards the corner, let's take the whole domain minus a small disk  $D_\rho$  centered at the corner (see fig.6). In particular the magnetic field satisfies the following equation:

$$\begin{aligned} -\text{div} \left( \frac{1}{\epsilon} \nabla u \right) &= \omega^2 \mu u && \text{in } \Omega / D_\rho \\ u &= 0 && \text{on } \partial\Omega \end{aligned} \quad (3)$$

By multiplying the equation by  $\bar{u}$  and integrating, after applying the Green's formula we obtain:

$$\int_{\Omega} \frac{1}{\epsilon} |\nabla u|^2 d\Omega - \int_{\partial D_\rho} \frac{1}{\epsilon} \frac{\partial u}{\partial n} \bar{u} d\Gamma = \omega^2 \int_{\Omega} |u|^2 d\Omega \quad (4)$$

Since  $u \in D(A_\gamma)$ , when  $\rho \rightarrow 0$ , one can assimilate the magnetic field to its asymptotic behaviour near the corner given by (2). After some calculus, one can check that the boundary term tends to  $-i\eta|\beta|^2(1 - |\gamma|^2) \int_{\theta=0}^{2\pi} \frac{1}{\epsilon} |\phi(\theta)|^2 d\theta$ . By taking the imaginary part of (4) we obtain for  $\rho \rightarrow 0$ :

$$-i\eta|\beta|^2(1 - |\gamma|^2) \int_{\theta=0}^{2\pi} \frac{1}{\epsilon} |\phi(\theta)|^2 d\theta = \text{Im}(\omega^2) \int_{\Omega} |u|^2 d\Omega \quad (5)$$

Despite the change of sign of  $\epsilon$ , one can prove the non trivial result:  $\eta \int_{\theta=0}^{2\pi} \frac{1}{\epsilon} |\phi(\theta)|^2 d\theta \geq 0$  [2]. Then  $\text{Im}(\omega^2)$  has the same sign as  $-|\beta|^2(1 - |\gamma|^2)$ . The equation (5) gives us lots of informations. Indeed, if we choose  $|\gamma| = 1$ , we see that  $\omega^2$  is real, which is coherent with the self-adjointness mentioned above. Let's take  $|\gamma| \neq 1$ . If  $\omega^2$  is real, then the left-hand side is equal to zero which implies that  $\beta = 0$  and  $u = u_A \in D(A)$ . It means that no real eigenvalue ( $\omega_i^2$ ) is exciting the singularity  $s_\gamma$ , so they correspond to the eigenvalues of the initial operator  $A$ . This wouldn't be the case for self-adjoint extensions. All the complex eigenvalues have the same sign for their imaginary

part: if  $|\gamma| > 1$  then  $\text{Im}(\omega^2) \geq 0$ , whereas if  $|\gamma| < 1$  then  $\text{Im}(\omega^2) \leq 0$ . For simplicity we choose here  $\gamma = 0$  such that the extended operator  $A_0$  takes only one singularity into account, and also  $\text{Im}(\omega_i^2) \leq 0 \quad \forall i$ . This singularity can be captured numerically using Perfectly Matched Layers (PMLs).

### An efficient numerical method to capture the black-hole waves

Usually, PMLs are used to bound infinite domains, for instance to truncate waveguides. Here we operate an original use of PMLs by putting them at the corners in order to capture the black-hole waves. Indeed, for each disk  $D_\rho$  centered at a corner, by the Euler change of variables  $(r, \theta) \mapsto (\log(r), \theta)$  we transform the disk into a semi-infinite waveguide:

$$\begin{aligned} -\text{div} \left( \frac{1}{\epsilon} \nabla u \right) &= \omega^2 \mu u \quad \text{in } D_\rho \quad (x, y) \\ &\Downarrow \\ -\frac{1}{\epsilon} \left( \frac{\partial u}{\partial r} \right)^2 - \frac{\partial}{\partial \theta} \left( \frac{1}{\epsilon} \frac{\partial u}{\partial \theta} \right) &= \omega^2 \mu r^2 u \quad \text{in } D_\rho \quad (r, \theta) \\ &\Downarrow z = \log\left(\frac{r}{\rho}\right) \\ -\text{div} \left( \frac{1}{\epsilon} \nabla u \right) &= \omega^2 \mu e^{2z} u \quad \text{in } ]-\infty, 0] \times [0, 2\pi] \quad (z, \theta) \end{aligned}$$

Then we use PMLs in a standard way. Basically, it consists in stretching the propagation direction  $z$  by a complex number  $\alpha$ ,  $\text{Re}(\alpha) > 0$ :

$$\begin{aligned} -\text{div} \left( \frac{1}{\epsilon} \nabla u \right) &= \omega^2 \mu e^{2z} u \quad \text{in } ]-\infty, 0] \times [0, 2\pi] \quad (z, \theta) \\ &\Downarrow z \rightarrow \frac{z}{\alpha} \\ -\frac{\alpha^2}{\epsilon} \frac{\partial^2 u}{\partial z^2} - \frac{\partial}{\partial \theta} \left( \frac{1}{\epsilon} \frac{\partial u}{\partial \theta} \right) &= \omega^2 \mu e^{2z/\alpha} u \quad \text{in } ]-\infty, 0] \times [0, 2\pi] \quad (z, \theta) \end{aligned}$$

When  $\alpha$  is suitably chosen, the asymptotic behaviour (2) leads to a sum of evanescent modes, even  $s^+$  (and a constant mode) such that we can truncate the waveguide at  $z = -L$ : we put a Neumann condition at  $z = -L$  to avoid reflexion of the constant mode. For an implementation point of view, we split the problem in two: the problem in the whole domain minus  $D_\rho$ , and the problem at the corner transformed into a strip. It requires matching conditions between the two solutions. Computations confirm that the PMLs' method is efficient to ensure the stability of the Finite Elements approximation. Note that the  $A_0$  spectrum contains complex eigenvalues which clearly proves its non self-adjointness. All the eigenvalues belong to  $\{z \in \mathbb{C} \text{ s.t. } \text{Im}(z) \leq 0\}$ , which is numerically almost satisfied (see fig.8).

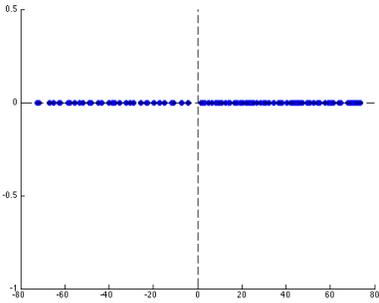


Figure 7: Spectrum of the SC. operator in the complex plane.

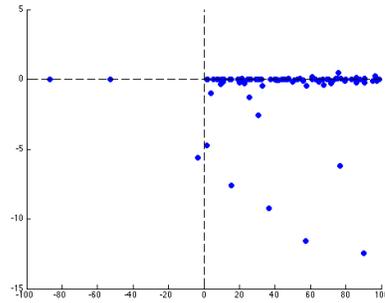


Figure 8: Spectrum of operator  $A_0$  in the complex plane.

#### 4. TOWARDS THE NON LINEAR EIGENVALUE PROBLEM

Considering the dispersionless Drude's model permittivity, one can rewrite the time-harmonic Maxwell equations for the Transverse Magnetic polarization as a non linear eigenproblem:

$$\begin{aligned} -\operatorname{div}\left(\frac{1}{\epsilon(\omega)}\nabla u\right) &= \omega^2\mu u && \text{in } \Omega \\ u &= 0 && \text{on } \partial\Omega \end{aligned} \quad (6)$$

with  $\epsilon(\omega) = \begin{cases} \epsilon_1 > 0 & \text{in } \Omega_1 \\ \epsilon_2(\omega) = \epsilon_\infty \left(1 - \frac{\omega_p^2}{\omega^2}\right) & \text{in } \Omega_2 \end{cases}$  where  $\omega_p$  is the plasma frequency,  $\epsilon_\infty > 0$  the limit behaviour of the metal at high frequencies: for  $\omega < \omega_p$ ,  $\epsilon_2(\omega) < 0$ . Let's write the variational formulation:

Find  $u \in H_0^1(\Omega)$  such that:

$$\frac{1}{\epsilon_1} \int_{\Omega_1} \nabla u \cdot \nabla \bar{v} \, d\Omega + \frac{1}{\epsilon_\infty} \frac{\omega^2}{\omega^2 - \omega_p^2} \int_{\Omega_2} \nabla u \cdot \nabla \bar{v} \, d\Omega = \omega^2 \int_{\Omega} u \bar{v} \, d\Omega \quad \forall v \in H_0^1(\Omega) \quad (7)$$

We multiply (7) by  $\omega^2 - \omega_p^2$  [6] and sort the terms. This leads to a polynomial equation in  $\omega$ :

$$\omega^4 \mathcal{M}_2(u, v) + \omega^2 \mathcal{M}_1(u, v) + \mathcal{M}_0(u, v) = 0$$

with

$$\begin{aligned} \mathcal{M}_0(u, v) &= \int_{\Omega} \tilde{\omega} \nabla u \cdot \nabla \bar{v} \, d\Omega, \quad \tilde{\omega} = \begin{cases} \frac{\omega_p^2}{\epsilon_1} & \text{in } \Omega_1 \\ 0 & \text{in } \Omega_2 \end{cases} \\ \mathcal{M}_1(u, v) &= \int_{\Omega} \frac{1}{\tilde{\epsilon}} \nabla u \cdot \nabla \bar{v} \, d\Omega + \omega_p^2 \int_{\Omega} u \bar{v} \, d\Omega, \quad \tilde{\epsilon} = \begin{cases} \epsilon_1 & \text{in } \Omega_1 \\ \epsilon_\infty & \text{in } \Omega_2 \end{cases} \\ \mathcal{M}_2(u, v) &= \int_{\Omega} u \bar{v} \, d\Omega \end{aligned}$$

One can reformulate this problem into a system with the two unknowns  $(u, w)$ ,  $w = \omega^2 u$ . After discretization, we obtain a linear eigenvalue problem:

$$\begin{pmatrix} \mathbb{M}_0 & 0 \\ 0 & \mathbb{I} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{w} \end{pmatrix} = \omega^2 \begin{pmatrix} -\mathbb{M}_1 & -\mathbb{M}_2 \\ \mathbb{I} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{w} \end{pmatrix} \quad (8)$$

which we can solve as the previous one. Recent works on computations with Finite Elements shows an accumulation point of the eigenvalues at 0 which seems coherent with [6].

#### ACKNOWLEDGMENT

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