Karlsruhe Institute of Technology

Wave phenomena
analysis and numerics

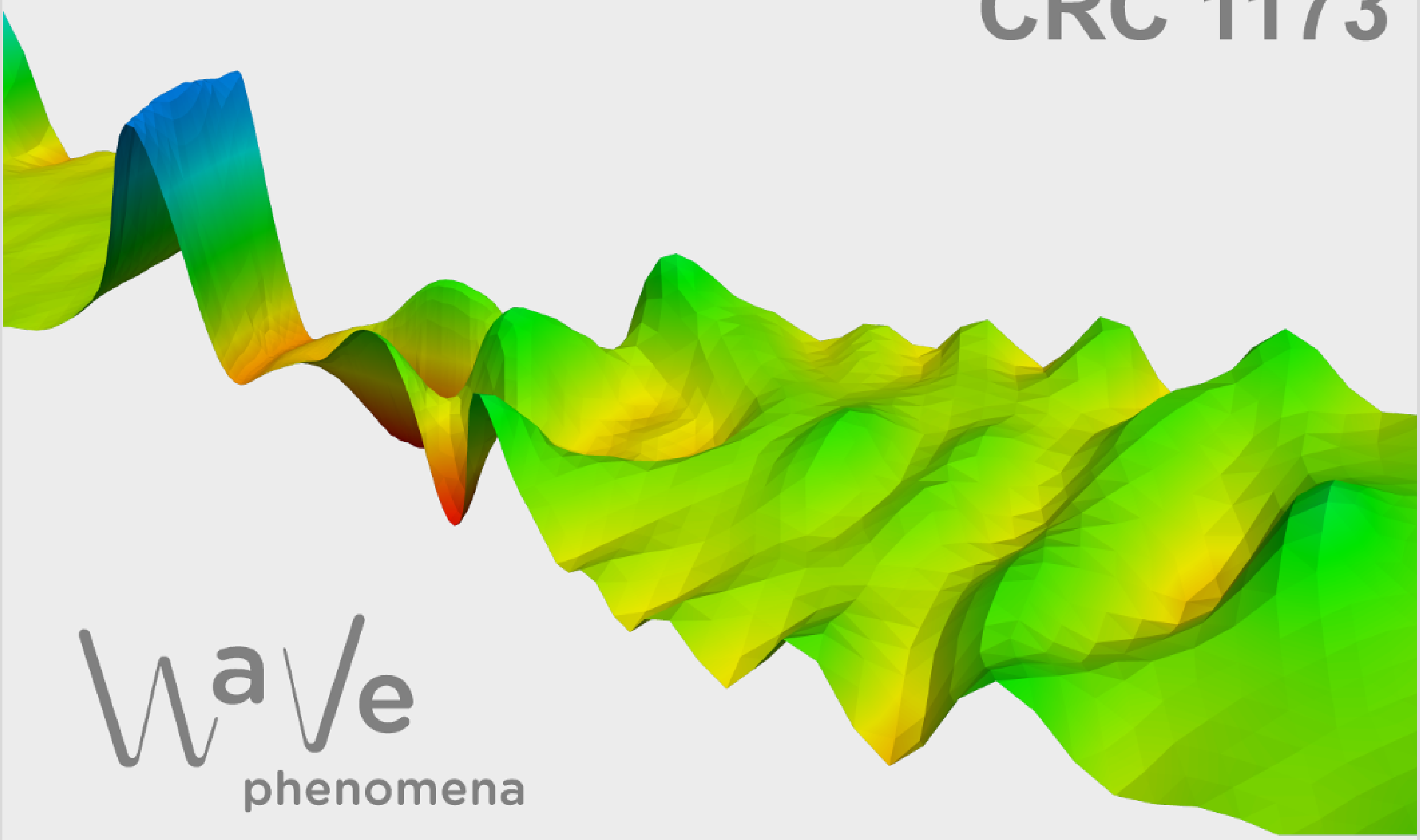
Scattering resonances in unbounded transmission problems with sign-changing coefficient

Camille Carvalho, Zoïs Moitier

CRC Preprint 2022/25, April 2022

KARLSRUHE INSTITUTE OF TECHNOLOGY

CRC 1173



Participating universities

Universität Stuttgart

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

TU WIEN

Funded by

DFG

ISSN 2365-662X

SCATTERING RESONANCES IN UNBOUNDED TRANSMISSION PROBLEMS WITH SIGN-CHANGING COEFFICIENT

CAMILLE CARVALHO AND ZOÏS MOITIER

Abstract. It is well-known that classical optical cavities can exhibit localized phenomena associated to scattering resonances (using the Black Box Scattering Theory), leading to numerical instabilities in approximating the solution. Those localized phenomena concentrate at the inner boundary of the cavity and are called whispering gallery modes. In this paper we investigate scattering resonances for unbounded transmission problems with sign-changing coefficient (corresponding to optical cavities with negative optical propertie(s), for example made of metamaterials). Due to the change of sign of optical properties, previous results cannot be applied directly, and interface phenomena at the metamaterial-dielectric interface (such as the so-called surface plasmons) emerge. We establish the existence of scattering resonances for arbitrary two-dimensional smooth metamaterial cavities. The proof relies on an asymptotic characterization of the resonances, and extending the Black Box Scattering Theory to problems with sign-changing coefficient. Our asymptotic analysis reveals that, depending on the metamaterial's properties, scattering resonances situated closed to the real axis are associated to surface plasmons. Examples for several metamaterial cavities are provided.

1. Introduction

Unbounded transmission problems with sign-changing coefficients arise in electromagnetics, in particular when one considers Maxwell's equations in the time harmonic regime (with Transverse Electric or Transverse Magnetic polarization) in dielectric-metamaterial structures (typically a bounded metamaterial cavity surrounded by a dielectric). Contrary to common materials, metamaterials such as the Negative-Index Metamaterials (NIM) exhibit unusual optical properties: for instance a real-valued negative effective dielectric permittivity and/or a negative effective permeability at some frequency range. There is a great interest in modeling metamaterial cavities to confine and control light. In particular, at optical frequencies, localized interface surface waves called surface plasmons can arise at dielectric-metamaterial interfaces [29]. The field of plasmonics is very active as surface plasmons offer strong light enhancement, with applications to next-generation sensors, antennas, high-resolution imaging, cloaking and other [40]. However, surface plasmons are very sensitive to the geometry and therefore challenging to capture, experimentally and numerically [8, 25]. Mathematically, surface plasmons are solutions of the homogeneous Maxwell's equations, they are oscillatory waves along the dielectric-metamaterial interface while exponentially decreasing in both transverse directions.

In classical transmission problems (meaning dielectric-dielectric structures), it has been shown that light can be confined by exciting the so-called Whispering Gallery Modes (WGM) [38]. WGM are essentially supported in the neighborhood of the interior cavity boundary and are associated to *scattering resonances* [6]. It is well-known that the approximation of light scattering in dielectric optical micro-cavities can be drastically affected by WGM, in particular if the excitation wavenumber of the source is close to

Date: April 21, 2022.

2010 *Mathematics Subject Classification.* 35P25, 35B40, 78A45.

Key words and phrases. Helmholtz Equation; Scattering resonances; Sign-changing coefficient; Asymptotic expansions.

a WGM resonance [32, 6]. In those cases the norm of the truncated resolvent operator explodes, which is observed numerically by the solution blowing-up (peaks): we call this *scattering instabilities*. Knowing the exact value of the scattering resonances is in general challenging (or impossible). However, one can obtain an asymptotic characterization of the scattering resonances, as done in [6].

The above results do not directly apply to metamaterial cavities due to the change of sign of the optical parameter(s) and the additional interface plasmonic behaviors. More precisely, well-posedness of the problem needs more attention, and spectral properties to define a *black box Hamiltonian* (including self-adjointness, lower semi-bound, etc.) may not be true. Also, surface plasmons have been mainly characterized and investigated in the context of the quasi-static approximation (e.g. [12, 23, 8, 4, 17, 14, 13]) — where an analytic expression can be found — therefore there is a need to obtain a characterization for the full problem (no quasi-static) to identify the associated metamaterial scattering resonances.

The goal of this paper is to establish those results for various two-dimensional metamaterial cavities (arbitrary smooth shape, with one arbitrary varying negative optical parameter). Using the $\mathtt{T}$-coercivity theory [10, 8, 9], and in the spirit of [6], we establish that the associated spectral operator of scalar transmissions problem with sign-changing coefficient is a black box Hamiltonian, and we carry out an asymptotic approximation of the metamaterial scattering resonances. In this case we find that there is an additional interface resonance family (compared to classical cavities) related to surface plasmons, and a specific scaling is required to asymptotically characterize them. This family can be located close to the real axis, and is responsible for scattering instabilities.

The paper is organized as follows. We present the problem and main results in Section 2. To illustrate the metamaterial scattering resonances and their effect, we provide a pedagogical example (case of a circular metamaterial cavity with constant negative coefficient) in Section 3. Section 4 presents the general approach for arbitrary metamaterial cavities, including the constructions of the asymptotic approximation at any order. Section 5 proves their connection to the truncated resolvent operator (extension of the Black Box Scattering Theory) and their consequence on scattering instabilities. Section 6 presents numerical illustrations of the metamaterial scattering resonances, and Section 7 presents our concluding remarks. Appendix A provides theoretical results about the problem operator, and Appendix B provides additional results and proofs needed in Section 4.

2. Problem setting and main result

2.1. Mathematical settings. Let us start by introducing the unbounded transmission problem with sign-changing coefficient, and its spectral analogous. We consider an open bounded connected set $\Omega \subset \mathbb{R}^2$ with smooth boundary $\Gamma = \partial\Omega$, that represents a transparent (penetrable) optical *cavity* characterized by $a_{\mathsf{c}} \in \mathscr{C}^\infty\left(\overline{\Omega}; (-\infty, 0)\right)$. The cavity is surrounded by a homogeneous background. We denote $a \in \mathrm{L}^\infty(\mathbb{R}^2)$ the piece-wise smooth function such that

$$a \equiv a_{\mathsf{c}} \text{ on } \Omega \qquad \text{and} \qquad a \equiv 1 \text{ on } \mathbb{R}^2 \setminus \overline{\Omega}. \tag{2.1}$$

We consider the problem: For $f \in \mathrm{L}^2_{\mathrm{comp}}(\mathbb{R}^2)$, $g \in \mathrm{H}^{\frac{1}{2}}(\Gamma)$, and $k \in \mathbb{C} \setminus \{0\}$, find $u \in \mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}^2)$ such that

$$\begin{cases} -\operatorname{div}\left(a^{-1}\,\nabla u\right) - k^2 u = f & \text{in } \mathbb{R}^2 \\ [u]_\Gamma = 0, \quad [a\,\partial_n u]_\Gamma = g & \text{across } \Gamma \\ u \quad k\text{-outgoing} & \end{cases} \tag{2.2}$$

and the associated spectral problem: Find $(\ell, u) \in \mathbb{C} \setminus \mathbb{R}_- \times \mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}^2)$ such that $u \not\equiv 0$ and

$$\begin{cases} -\operatorname{div}\left(a^{-1}\nabla u\right) = \ell^2 u & \text{in } \mathbb{R}^2 \\ [u]_\Gamma = 0, \quad [a\,\partial_n u]_\Gamma = 0 & \text{across } \Gamma\,. \\ u \quad \ell\text{-outgoing} \end{cases} \tag{2.3}$$

Above, $\mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}^2) := \left\{u \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^2) \;\middle|\; \forall \chi \in \mathscr{C}^\infty_{\mathrm{comp}}(\mathbb{R}^2),\ \chi u \in \mathrm{H}^1(\mathbb{R}^2)\right\}$ and $n : \Gamma \to \mathbb{S}^1$ is the unit normal vector outward to Ω. Given X, we denote $[X]_\Gamma(\gamma) = \lim_{x\to\gamma^+} X(x) - \lim_{x\to\gamma^-} X(x)$, for any $\gamma \in \Gamma$, the jump condition across Γ. The jump conditions $[u]_\Gamma = 0$ and $[a\,\partial_n u]_\Gamma = 0$ will be referred to as the *transmission conditions*. We say that v is *k-outgoing* if it satisfies the outgoing wave condition:

$$v(r,\theta) = \sum_{m\in\mathbb{Z}} w_m(r)\,\mathrm{e}^{\mathrm{i}m\theta} = \sum_{m\in\mathbb{Z}} c_m\,\mathsf{H}^{(1)}_m(kr)\,\mathrm{e}^{\mathrm{i}m\theta} \tag{2.4}$$

with polar coordinates (r,θ) such that $r > \sup_{x\in\Omega}|x|$, $\theta \in \mathbb{R}/2\pi\mathbb{Z}$, $\mathsf{H}^{(1)}_m$ the Hankel function of the first kind of order m, and $(c_m)_{m\in\mathbb{Z}} \in \mathbb{C}^{\mathbb{Z}}$. For a pair (ℓ, u) solution of Eq. (2.3), ℓ is called a *scattering resonance* and the function u is a *resonant mode* associated to ℓ.

We define $P : u \mapsto -\operatorname{div}(a^{-1}\nabla u)$ the $\mathrm{L}^2(\mathbb{R}^2)$ operator from Eq. (2.3) with the domain $\mathcal{D}(P) := \{u \in \mathrm{L}^2(\mathbb{R}^2) \mid -\operatorname{div}(a^{-1}\nabla u) \in \mathrm{L}^2(\mathbb{R}^2)\}$[1]. We also define the local version of the domain $\mathcal{D}_{\mathrm{loc}}(P) := \left\{u \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^2) \;\middle|\; \forall\chi \in \mathscr{C}^\infty_{\mathrm{comp}}(\mathbb{R}^2),\ \chi u \in \mathcal{D}(P)\right\}$.

For classical cavities ($a_{\mathsf{c}} > 0$), one can show that Eq. (2.2) is well-posed in $\mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}^2)$, the operator $(P, \mathcal{D}(P))$ is self-adjoint, its spectrum is real and admits a lower bound. This allows us in particular to work in the framework of the *black box scattering* [20, Definition. 4.6], where one can check that there is an underlying *black box Hamiltonian* (see Lemma 5.2 for more details). We can define $\mathfrak{Res} : k \mapsto (P - k^2)^{-1}$ the resolvent[2] associated to P. An asymptotic characterization of the scattering resonances close to the real axis (called *quasi-resonances* $\underline{k}_m$) is provided in [6], and with the black box scattering theory it is proved that true resonances $(\ell_m)_m$ are super-algebraically close to quasi-resonances $\underline{k}_m$. As a consequence the solution of Eq. (2.2) blows-up for $k = \underline{k}_m$ (and the norm of the truncated resolvent $\mathfrak{Res}(\underline{k}_m)$ explodes).

Due to the change of sign of a, the black box scattering theory doesn't directly apply in our case. First, well-posedness is not guaranteed as $\mathsf{P} : \mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}^2) \to \mathrm{H}^{-1}_{\mathrm{loc}}(\mathbb{R}^2)$, $\mathsf{P}u = -\operatorname{div}(a^{-1}\nabla u)$ is not necessarily a Fredholm operator (or in other words the coercivity of the associated weak form of Eq. (2.2) is not guaranteed). Additionally, spectral requirements on P to be a black box Hamiltonian are not obvious. Finally, it is not clear whether there exist resonances close to the real axis that are associated to localized interface modes (potentially related to surface plasmons).

The goal of this paper is to extend the black box scattering framework and to provide an asymptotic characterization of scattering resonances to unbounded transmission problems with sign-changing coefficient.

Remark 2.1.

- The k-outgoing condition defined in Eq. (2.4) is equivalent to v satisfying the so-called Sommerfeld radiation condition if, and only if, $k > 0$. This outgoing condition is more general, and will be also used for the associated spectral problem, where one can have $k \in \mathbb{C}$.

---

[1] One can show that $\mathcal{D}(P) = \left\{u \in \mathrm{H}^1(\mathbb{R}^2) \;\middle|\; u|_\Omega \in \mathrm{H}^2(\Omega),\ u|_{\mathbb{R}^2\setminus\overline{\Omega}} \in \mathrm{H}^2(\mathbb{R}^2 \setminus \overline{\Omega}),\ \left[a^{-1}\partial_n u\right]_\Gamma = 0\right\}$. This second definition will be heavily used in Section 4, Section 5.

[2] $\mathfrak{Res}$ is defined on the first quadrant of the complex plane ($\Re(k) > 0$ and $\Im(k) > 0$). Using the *black box scattering* framework (see [20]), we can extend the resolvent to $\mathbb{C} \setminus \mathbb{R}_-$.

- Depending on the polarization (TE / TM), the optical cavity is characterized by a permittivity $a = \varepsilon$ and a permeability $\mu = 1$ or a permeability $a = \mu$ and a permittivity $\varepsilon = 1$. Metamaterials are commonly characterized by $\varepsilon < 0$ and/or $\mu < 0$. The cavity is embedded in a homogeneous background characterized by $\mu = 1$, and $\varepsilon = 1$.
- Equation (2.2) includes the scattering by a plane wave.

2.2. **Main result.** Our main goal is to establish the existence of a discrete sequence of scattering resonances close to the positive real axis, which is done in two steps. First, we derive approximate solutions of the resonance problem Eq. (2.3) called *quasi-pairs* [6, Definition. 2.1] (Theorem 2.3); then we show that there exist true resonances close to the approximate ones (Theorem 2.4), which rely on extending the black box scattering theory for Eq. (2.3). For ease of reading, we (re)define quasi-pairs as follows:

Definition 2.2. A *quasi-pair* for the resonance problem Eq. (2.3) is formed by a sequence $(\underline{\lambda}_m)_{m\geq 1}$ of real numbers, and a sequence $(\underline{u}_m)_{m\geq 1}$ of complex valued functions that satisfy the following conditions:

(1) For any $m \geq 1$, the functions $\underline{u}_m$ are uniformly compactly supported and
$$\underline{u}_m \in \mathcal{D}(P), \quad \text{with} \quad \|\underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = 1.$$
(2) We have the following quasi-pair estimate
$$\|P\underline{u}_m - \underline{\lambda}_m \underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}\left(m^{-\infty}\right), \qquad \text{as } m \to +\infty, \tag{2.5}$$
with the notation $a_m = \mathcal{O}(m^{-\infty})$ to indicate that for all $N \in \mathbb{N}$, there exists $C_N > 0$ such that $|a_m| \leq C_N\, m^{-N}$, for all $m \geq 1$.

(3) Additionally, we say that $\underline{u}_m$ is localized around $\Gamma \subset \mathbb{R}^2$ if, for all $\delta > 0$, its support is mainly in $\Gamma_\delta := \{x \in \mathbb{R}^2 \mid \operatorname{dist}(x, \Gamma) < \delta\}$ neighborhood of Γ in the sense that
$$\|\underline{u}_m\|_{\mathrm{L}^2(\Gamma_\delta)} = 1 - \mathcal{O}\left(m^{-\infty}\right), \qquad \text{as } m \to +\infty. \tag{2.6}$$

We call $(\underline{u}_m)_{m\geq 1}$ quasi-modes, and $\left(\underline{k}_m := \sqrt{\underline{\lambda}_m}\right)_{m\geq 1}$ quasi-resonances.

Theorem 2.3. *If $a_{\mathsf{c}}(\gamma) \neq -1$, for all $\gamma \in \Gamma$, then we can construct $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$ quasi-pairs of the resonance problem Eq. (2.3) Moreover, we have $\underline{\lambda}_m = \left(\frac{2\pi m}{L}\right)^2 \Lambda\left(\frac{L}{2\pi m}\right)$ where L is the length of the curve Γ and $\Lambda \in \mathscr{C}^\infty\left(\left[0, \frac{L}{2\pi}\right]\right)$ (see Eq. (4.16a)). The quasi-mode is of the form $\underline{u}_m = \exp\left(\mathrm{i}\frac{2\pi m}{L}\Theta\right)\Phi$ with Θ, Φ smooth functions with respect to $\frac{L}{2\pi m}$ and Φ is exponentially decreasing on both sides of the interface Γ (see Eq. (4.16b)). Additionally, the sign of $\underline{\lambda}_m$ is given to leading order by the sign of $1 + a_{\mathsf{c}}|_\Gamma^{-1}$, and $(\underline{\lambda}_m)_{m\geq 1}$ are independent of the construction.*

Theorem 2.4. *If $a_{\mathsf{c}}(\gamma) \neq -1$, for all $\gamma \in \Gamma$, let $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$ be the quasi-pairs of Theorem 2.3. Then there exists a sequence of true scattering resonances $(\ell_m)_{m\geq 1}$ of Eq. (2.3) close to the quasi-resonances $\left(\sqrt{\underline{\lambda}_m}\right)_{m\geq 1}$ in the sense that*
$$\ell_m^2 = \underline{\lambda}_m + \mathcal{O}\left(m^{-\infty}\right), \qquad \text{as } m \to +\infty.$$
In addition:

- *If $a(\gamma) < -1$, for all $\gamma \in \Gamma$, then $(\ell_m)_{m\geq 1}$ are scattering resonances with $\Re\left(\ell_m^2\right) > 0$ and $-1 \ll \Im\left(\ell_m^2\right) < 0$.*
- *If $-1 < a(\gamma) < 0$, for all $\gamma \in \Gamma$, then $(\ell_m)_{m\geq 1}$ are scattering resonances with $\Re\left(\ell_m^2\right) < 0$ and $-1 \ll \Im\left(\ell_m^2\right) \leq 0$.*

Contrary to the classical cavities ($a_{\mathsf{c}} > 0$), the value of a_{c} can lead to two different behaviors: from Theorem 2.3 we only have one sequence of resonances close to the positive real axis in the case $a(\gamma) < -1$ (where $(\underline{k}_m)_m \in \mathbb{R}$), and none in the case $-1 < a(\gamma) < 0$

(where $(\underline{k}_m)_m \in \mathrm{i}\mathbb{R}$), see [33, 6]. From Theorem 2.4 one can show that the truncated resolvent explodes at the quasi-resonances, and thus scattering instabilities occur for Eq. (2.2).

Corollary 2.5. *If $a(\gamma) < -1$, for all $\gamma \in \Gamma$, then there exists a real sequence $(\underline{k}_m)_{m\geq 1}$ with $\lim_{m\to+\infty} \underline{k}_m = +\infty$ such that for all $\chi \in \mathscr{C}^{\infty}_{\mathrm{comp}}(\mathbb{R}^2)$ with $\chi \equiv 1$ on an open neighborhood of $\overline{\Omega}$ and for all $N \in \mathbb{N}$, there exists a constant $C_N > 0$,*

$$\|\!|\chi \mathfrak{Res}(\underline{k}_m)\chi\|\!| \geq C_N m^N, \qquad \forall m \geq 1.$$

The above results also rely on well-posedness of Eq. (2.2), and on establishing that P is a black box Hamiltonian. This can be done using the T-coercivity framework [10, 8, 9], allowing to compensate for the change of sign of a and establishing Fredholm properties (and others) under some conditions. Section 5 and Appendix A detail those results. Well-posedness of Eq. (2.2) in Hadamard's sense leads to the existence of a stability constant $C(k) > 0$ such that $\|u\|_{\mathrm{L}^2} \leq C(k) \left(\|f\|_{\mathrm{L}^2} + \|g\|_{\mathrm{L}^2(\Gamma)}\right)$ (see Lemma A.2). From Corollary 2.5 we deduce the following:

Corollary 2.6. *If $a(\gamma) < -1$, for all $\gamma \in \Gamma$, then there exists a real sequence $(\underline{k}_m)_{m\geq 1}$ with $\lim_{m\to+\infty} \underline{k}_m = +\infty$ such that for all $N \in \mathbb{N}$, there exists a constant $C_N > 0$,*

$$C(\underline{k}_m) \geq C_N m^N, \qquad \forall m \geq 1.$$

Equation (2.2) suffers from scattering instabilities for $k = \underline{k}_m$.

The construction of the real sequence $(\underline{\lambda}_m)_m$ (consequently $(\underline{k}_m)_m$) is the fundamental element in the above results. To illustrate how to proceed, we present a simple case in Section 3 where all calculations can be done explicitly, and we generalize the approach to arbitrary smooth cavities in Section 4.

3. A pedagogical example

In this section we consider Eq. (2.2) set on a circular cavity with constant negative a_{c}: Ω is a disk of radius $R > 0$, and $a_{\mathsf{c}} = -\eta^2$ with $\eta > 0$. Taking advantage of the geometry, we look for solution of the form:

$$u(x) = u(r,\theta) = \sum_{m\in\mathbb{Z}} u_m(r,\theta) = \sum_{m\in\mathbb{Z}} w_m(r)\,\mathrm{e}^{\mathrm{i}m\theta}, \tag{3.1}$$

with $(r,\theta) \in \mathbb{R}_+ \times \mathbb{R}/2\pi\mathbb{Z}$ the polar coordinates corresponding to the Cartesian coordinates x, and $w_m(r) = \frac{1}{2\pi}\int_0^{2\pi} u(r,\theta)\,\mathrm{e}^{-\mathrm{i}m\theta}\,\mathrm{d}\theta$, $m \in \mathbb{Z}$, the angular Fourier coefficients. Similarly, we assume we can write $f(x) = \sum_{m\in\mathbb{Z}} f_m(r)\,\mathrm{e}^{\mathrm{i}m\theta}$, for $x \in \mathbb{R}^2$ with $f_m \in \mathrm{L}^2_{\mathrm{comp}}(\mathbb{R})$, and we can write $g(x) = \sum_{m\in\mathbb{Z}} g_m\,\mathrm{e}^{\mathrm{i}m\theta}$, for $x \in \Gamma$ with $g \in \mathrm{H}^{\frac{1}{2}}(\Gamma)$.

Remark 3.1. An example where Eq. (2.2) naturally arises is the scattering by a transparent obstacle of a plane wave. If one considers $u^{\mathsf{in}}(x_1,x_2) = \mathrm{e}^{\mathrm{i}kx_2}$, with wavenumber k and direction $(0,1)^{\mathsf{T}}$, then Eq. (2.2) is satisfied by the scattered field $u^{\mathsf{sc}} := u - u^{\mathsf{in}}$ with data $f^{\mathsf{in}} := \operatorname{div}\left(a^{-1}\,\nabla u^{\mathsf{in}}\right) + k^2 u^{\mathsf{in}}$ and $g^{\mathsf{in}} := -\left[a^{-1}\,\partial_n u^{\mathsf{in}}\right]_\Gamma$. Additionally, one can check that f_m is supported only in the cavity: $f_m(r) = k^2(a_{\mathsf{c}} - 1)\,\mathsf{J}_m(k\,r)$, $r \in (0,R)$, where J_m denotes the Bessel function of the first kind of order m. This expansion is obtained using the Jacobi-Anger expansion of u^{in} [37, Eq. 10.12.1] that converges absolutely on every compact set of $\mathbb{R}^2$.

Plugging Eq. (3.1) in Eq. (2.2), we obtain a family of 1D problems indexed by $m \in \mathbb{Z}$: Find $w_m \in \mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}_+, r\,\mathrm{d}r)$ such that

$$\begin{cases} -\dfrac{1}{r}\partial_r\left(r\,\partial_r w_m\right) + \dfrac{m^2}{r^2} w_m - a_{\mathsf{c}} k^2\, w_m = f_m & \text{in } (0,R) \\ -\dfrac{1}{r}\partial_r\left(r\,\partial_r w_m\right) + \dfrac{m^2}{r^2} w_m - k^2\, w_m = f_m & \text{in } (R,+\infty) \\ \left[a^{-1}\, {w_m}'\right]_{\{R\}} = g_m & \text{across } \{R\} \\ {w_0}'(0) = 0 \quad \text{or} \quad w_m(0) = 0 \text{ for } m \neq 0 & \text{on } \{0\} \\ w_m(r) \propto \mathsf{H}^{(1)}_m(kr) & r > R \end{cases} \tag{3.2}$$

with $\propto$ meaning "up to a constant". For $m \neq 0$, the term $\frac{m^2}{r^2} w_m$ imposes a homogeneous Dirichlet boundary condition at zero [7]. The solution is continuous at $r = 0$, using the outgoing wave condition we write

$$w_m(r) = \begin{cases} \alpha_m \dfrac{\mathsf{I}_m(\eta\, k\, r)}{\mathsf{I}_m(\eta\, k\, R)} + f_{a_{\mathsf{c}}}(r) & \text{if } r \leq R \\ \beta_m \dfrac{\mathsf{H}^{(1)}_m(k\, r)}{\mathsf{H}^{(1)}_m(k\, R)} + f_R(r) & \text{if } r > R \end{cases} \tag{3.3}$$

with I_m denoting the modified Bessel function of the first kind of order m, and $f_{a_{\mathsf{c}}}, f_R$ denoting particular solutions. Our goal in this section is to investigate the associated operator (in particular the resolvent operator), therefore we do not need to write the particular solutions explicitly. Above, the coefficients (α_m, β_m) are solution of

$$A^\eta_m(kR)\begin{pmatrix}\alpha_m \\ \beta_m\end{pmatrix} = \begin{pmatrix} f_{a_{\mathsf{c}}}(R) - f_R(R) \\ g_m + {a_{\mathsf{c}}}^{-1} f'_{a_{\mathsf{c}}}(R) - f'_R(R)\end{pmatrix}, \quad A^\eta_m(z) = \begin{pmatrix} 1 & -1 \\ -\frac{1}{\eta}\frac{\mathsf{I}'_m(\eta\, z)}{\mathsf{I}_m(\eta\, z)} & -\frac{{\mathsf{H}^{(1)}_m}'(z)}{\mathsf{H}^{(1)}_m(z)}\end{pmatrix}. \tag{3.4}$$

The above system comes from the transmission conditions at $r = R$.

Remark 3.2. Since $k > 0$ and the problem is well-posed for $\eta \neq 1$ (see Lemma A.2), coefficients (α_m, β_m) are uniquely defined and $\det(A^\eta_m(kR)) \neq 0$, with

$$\det(A^\eta_m(z)) \coloneqq -\eta^{-1}\frac{\mathsf{I}'_m(\eta\, z)}{\mathsf{I}_m(\eta\, z)} - \frac{{\mathsf{H}^{(1)}_m}'(z)}{\mathsf{H}^{(1)}_m(z)}, \quad \forall z \in \mathbb{C}^*. \tag{3.5}$$

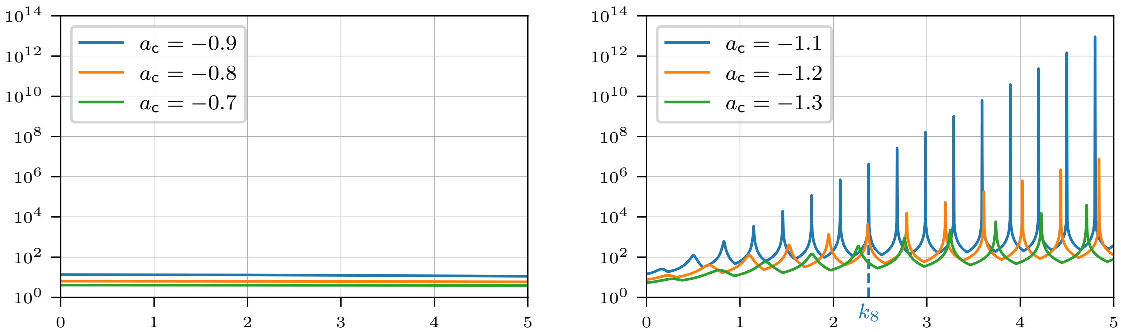
Now that we have an explicit expression of $(A^\eta_m(kR))_{m\in\mathbb{Z}}$, we can analyze its behavior for various wavenumbers k and values of a_{c} (namely η). For numerical purposes, we truncate Eq. (3.1) to order M, leading to consider the sequence of operators $\left(A^\eta_{-M}(kR), \ldots, A^\eta_0(kR), \ldots, A^\eta_M(kR)\right)$. We choose here $M = 32$ and $R = 1$. The resolvent of this spectral numerical scheme is $\mathbb{A}_k^{-1}$ where

$$\mathbb{A}_k \coloneqq \operatorname{diag}\left(A^\eta_{-M}(kR), \ldots, A^\eta_0(kR), \ldots, A^\eta_M(kR)\right). \tag{3.6}$$

To look at the stability of this scheme, we look at the spectral norm of $\mathbb{A}_k^{-1}$ noted $|||\mathbb{A}_k^{-1}|||_2$. Figure 1 represents the log plot of $|||\mathbb{A}_k^{-1}|||_2$ with respect to k, for various values of a_{c}. One observes that $|||\mathbb{A}_k^{-1}|||_2$ remains bounded when $a_{\mathsf{c}} \in (-1, 0)$, while there exists a sequence $(k_m)_m$ such that $|||\mathbb{A}_{k_m}^{-1}|||_2$ peaks when $a_{\mathsf{c}} \in (-\infty, -1)$. In the latter, the sequence $\left(|||\mathbb{A}_{k_m}^{-1}|||_2\right)_{m\geq 1}$ grows exponentially [32, 26]. We refer to those peaks as *scattering instabilities.*

The above results provide the following:

- While Eq. (2.2) is well-posed for all $k > 0$, the associated resolvent operator explodes for a sequence of wavenumbers $(k_m)_{m\geq 1}$.



$a_c \in \{-0.9, -0.8, -0.7\}$ $a_c \in \{-1.3, -1.2, -1.1\}$

Figure 1. *Semi-log plot of the function* $k \mapsto |||\mathbb{A}_k^{-1}|||_2$ *with respect to* k *for* $a_c \in \{-0.9, -0.8, -0.7\}$ *(left), for* $a_c \in \{-1.3, -1.2, -1.1\}$ *(right). The value* k_8 *marked on the graph corresponds to the reference value used in Figs. 4 and 5.*

- This phenomenon occurs only for $a_c < -1$.

In what follows we investigate the associated spectral problem to identify the resonances causing the scattering instabilities. We then use semi-classical analysis to characterize the sequence $(k_m)_{m\geq 1}$, and study their relationship to surface plasmons.

3.1. **Scattering resonances for the disk.** As done in the previous section, Eq. (2.3) set on a disk can be rewritten as a family of one-dimensional problems indexed by $m \in \mathbb{Z}$: Find $(\ell, w_m) \in \mathbb{C} \setminus \mathbb{R}_- \times \mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}_+, r\,\mathrm{d}r) \setminus \{0\}$, such that

$$\begin{cases} -\dfrac{1}{r}\partial_r\left(r\,\partial_r w_m\right) + \dfrac{m^2}{r^2} w_m - a_c \ell^2\, w_m = 0 & \text{in } (0,R) \\ -\dfrac{1}{r}\partial_r\left(r\,\partial_r w_m\right) + \dfrac{m^2}{r^2} w_m - \ell^2\, w_m = 0 & \text{in } (R,+\infty) \\ \left[a^{-1}\, w_m'\right]_{\{R\}} = 0 & \text{across } \{R\} \\ {w_0}'(0) = 0 \quad \text{or} \quad w_m(0) = 0 \text{ for } m \neq 0 & \text{on } \{0\} \\ w_m(r) \propto \mathsf{H}^{(1)}_m(\ell r) & r > R \end{cases} \tag{3.7}$$

Similarly, we write

$$w_m(r) = \begin{cases} \alpha_m \dfrac{\mathsf{I}_m(\eta\,\ell\, r)}{\mathsf{I}_m(\eta\,\ell\, R)} & \text{if } r \leq R \\ \beta_m \dfrac{\mathsf{H}^{(1)}_m(\ell\, r)}{\mathsf{H}^{(1)}_m(\ell\, R)} & \text{if } r > R \end{cases} \tag{3.8}$$

however this time, the pair (ℓ, w_m) is solution of Eq. (3.7) if, and only if, there exists $(\alpha_m, \beta_m)^\intercal \in \ker\left(A^\eta_m(\ell R)\right) \setminus (0,0)^\intercal$, with $A^\eta_m(\ell R)$ defined in Eq. (3.4). Given $m \in \mathbb{Z}$, and using Eq. (3.5), we define the set of resonances

$$\mathcal{R}[a_c, R](m) = \left\{ \ell \in \mathbb{C} \setminus \mathbb{R}_- \;\middle|\; \det\left(A^\eta_m(\ell R)\right) = 0 \text{ and } -\frac{\pi}{2} < \arg(\ell) \leq \frac{\pi}{2} \right\}. \tag{3.9}$$

Finally, we define the set of resonances of Problem Eq. (2.3)

$$\mathcal{R}[a_c, R] := \bigcup_{m\in\mathbb{Z}} \mathcal{R}[a_c, R](m). \tag{3.10}$$

Remark 3.3. Given $\ell \in \mathcal{R}[a_c, R](m)$, one finds $\alpha_m = c$ and $\beta_m = c$ with $c \in \mathbb{C}^*$ since the resonant modes are defined up to some normalization.

Remark 3.4. Since $\mathsf{I}_{-m} = \mathsf{I}_m$ and $\mathsf{H}^{(1)}_{-m} = (-1)^m \mathsf{H}^{(1)}_m$, for all $m \in \mathbb{Z}$, see [37, Eq. 10.27.1 and 10.4.2], by symmetry all the resonances ℓ, corresponding to $m \neq 0$, are of multiplicity 2, and the two associated modes are conjugate, given by $u_m(r, \theta) := w_m(r)\, \mathrm{e}^{\pm i m \theta}$. It turns out $\mathcal{R}[a_\mathsf{c}, R] = \bigcup_{m \in \mathbb{N}} \mathcal{R}[a_\mathsf{c}, R](m)$.

The resonances set $(\mathcal{R}[a_\mathsf{c}, R](m))_m$ defined in Eq. (3.9) cannot be computed analytically, however one can use contour integration techniques on Eq. (3.5) to compute a subset $\mathcal{R}_N[a_\mathsf{c}, R] := \bigcup_{m=0}^{N} \mathcal{R}[a_\mathsf{c}, R](m) \subset \mathcal{R}[a_\mathsf{c}, R]$ (see [28, 39]). Figure 2 represents the set $\mathcal{R}_{64}[a_\mathsf{c}, 1]$ for the unit disk and for various permittivities a_c. The color bar indicates the value of m.

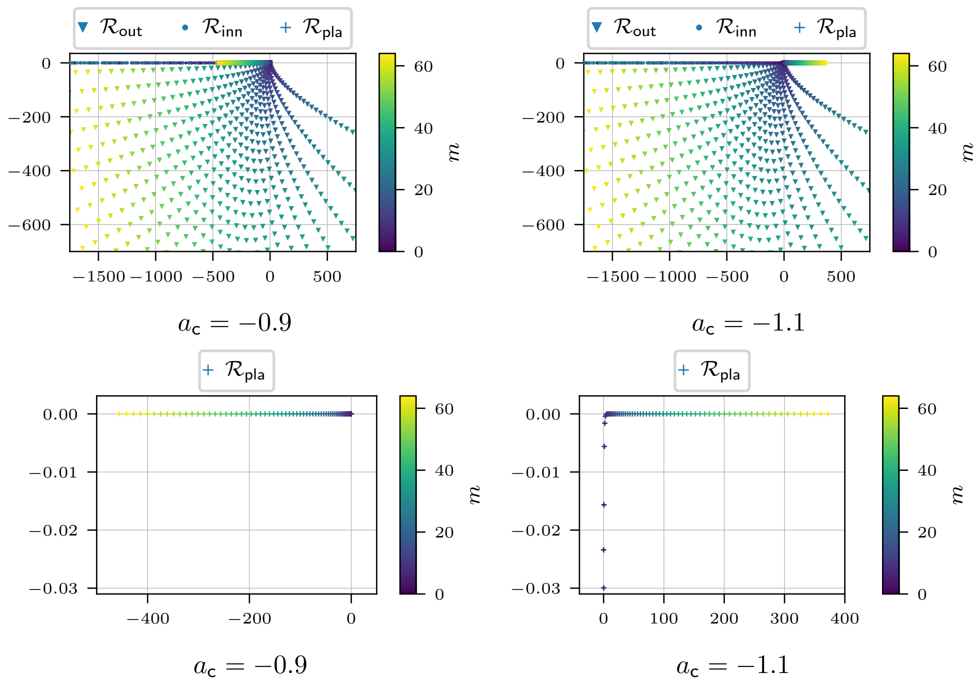
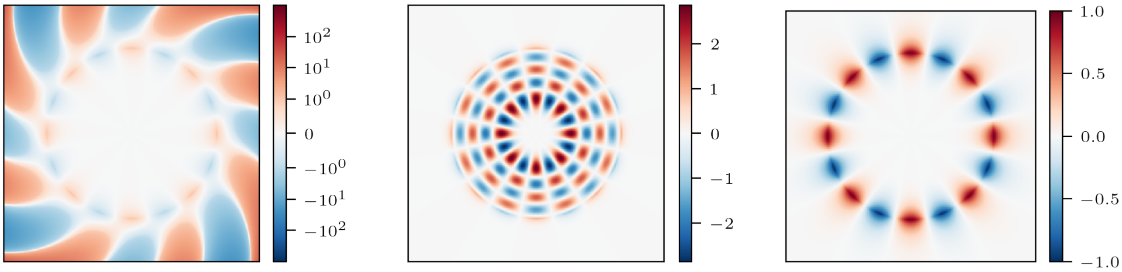


Figure 2. *Graph of the sets* $\mathcal{R}_{64}[-0.9, 1]$ *(left column) and* $\mathcal{R}_{64}[-1.1, 1]$ *(right column) in the complex plane* $(\Re(\ell^2), \Im(\ell^2))$*, the bottom row is a zoom on the interface resonances. Those sets are computed using complex contour integration* [39] *on the analytic function* Eq. (3.5)*.*

In classical cavities ($a_\mathsf{c} > 0$), resonances of Eq. (2.3) are split into two categories (at least for $a_\mathsf{c} > 1$ [6]): inner resonances $\mathcal{R}_{\mathsf{inn}}[a_\mathsf{c}, R]$ associated to resonant modes essentially supported inside the cavity Ω, and outer resonances $\mathcal{R}_{\mathsf{out}}[a_\mathsf{c}, R]$ associated to resonant modes essentially supported in the exterior of the cavity $\mathbb{R}^2 \setminus \overline{\Omega}$. The inner resonance category includes the so-called *Whispering Gallery Modes* (WGM), associated to resonances ℓ_{WGM} such that $-1 \ll \Im(\ell_{\mathrm{WGM}}) < 0$ [18, 6]. In particular the approximation of Eq. (2.2) can be deteriorated if one chooses $k = \Re(\ell_{\mathrm{WGM}})$, where those modes can be excited [32, Sec. 6.2]. When $a_\mathsf{c} < 0$ we split the resonances into three categories. From Figs. 2 to 4, we conclude:

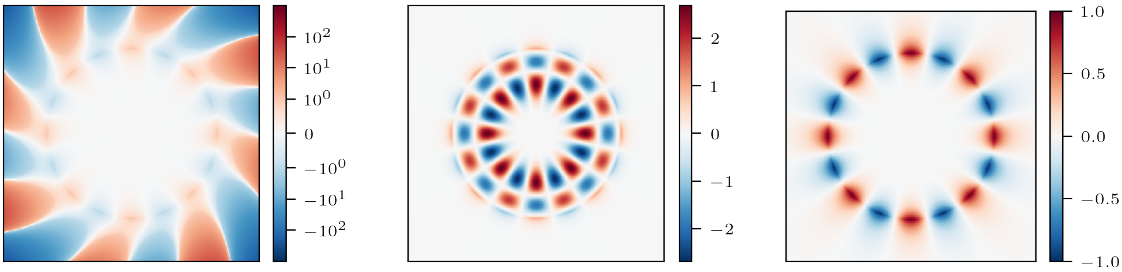
- The outer resonances $\mathcal{R}_{\mathsf{out}}[a_\mathsf{c}, 1]$ (represented as triangles in Fig. 2) are resonances with a negative imaginary part. The outer resonant modes are essentially supported outside the cavity.
- The inner resonances $\mathcal{R}_{\mathsf{inn}}[a_\mathsf{c}, 1]$ (represented as dots in Fig. 2) are pure imaginary eigenvalues of the operator P on $\mathrm{L}^2(\mathbb{R}^2)$ (consequently $\Re(\ell_{\mathsf{inn}}^2) < 0$). They contain whispering gallery modes. Inner resonances can be seen as outer resonances from the *inverted* cavity problem ($a_\mathsf{c} = 1$ and $a = -\eta^{-2}$ outside).

- The resonances represented by '+' in Fig. 2 (a zoom is provided Fig. 2c, Fig. 2d) are associated to resonant modes essentially supported on the interface Γ (see Fig. 5 for an example). We refer to those modes as surface plasmons waves (SPW), and we call this family the interface resonances $\mathcal{R}_{\mathsf{pla}}[a_{\mathsf{c}}, 1]$. We denote the interface resonances $(\ell_m)_{m\geq 1}$ so that $\mathcal{R}_{\mathsf{pla}}[a_{\mathsf{c}}, 1] = \{\ell_m \mid m \in \mathbb{N}^*\}$.



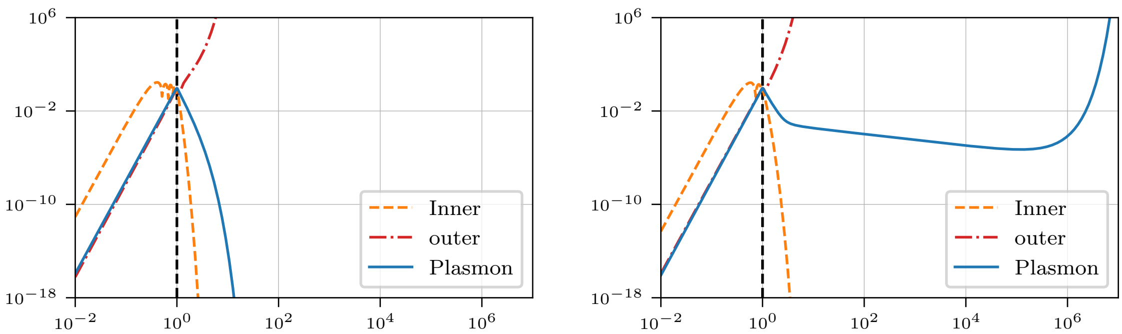
$\ell_{\mathsf{out}} \approx 5.229 - \mathrm{i}2.664$ $\ell_{\mathsf{inn}} \approx \mathrm{i}25.013$ $\ell_8 \approx \mathrm{i}2.664$

Figure 3. *Real part of some resonant modes $u_8(r, \theta)$ for $a_{\mathsf{c}} = -0.9$ with their corresponding resonances below.*



$\ell_{\mathsf{out}} \approx 3.174 - \mathrm{i}4.129$ $\ell_{\mathsf{inn}} \approx \mathrm{i}15.965$ $\ell_8 \approx 2.377 - \mathrm{i}4.194 \cdot 10^{-6}$

Figure 4. *Real part of some resonant modes $u_8(r, \theta)$ for $a_{\mathsf{c}} = -1.1$ with their corresponding resonances below.*



$a_{\mathsf{c}} = -0.9$ $a_{\mathsf{c}} = -1.1$

Figure 5. *Log-Log plots of the radial component $r \mapsto w_8(r)$ of the three types of resonances shown in Figs. 3 and 4 for $a_{\mathsf{c}} = -0.9$ (left) and $a_{\mathsf{c}} = -1.1$ (right).*

In the end, we write $\mathcal{R}[a_{\mathsf{c}}, R] = \mathcal{R}_{\mathsf{out}}[a_{\mathsf{c}}, R] \cup \mathcal{R}_{\mathsf{inn}}[a_{\mathsf{c}}, R] \cup \mathcal{R}_{\mathsf{pla}}[a_{\mathsf{c}}, R]$. The interface resonances are quite peculiar as their nature changes depending on a_{c}. As illustrated in Fig. 2, they are (for most cases imaginary) resonances such that $\Re(\ell_m^2) < 0$ when $-1 < a_{\mathsf{c}} < 0$, while they correspond to complex resonances such that $\Re(\ell_m^2) > 0$ when

$a_{\mathsf{c}} < -1$. For the latter, one observes that their real part diverges towards $+\infty$ as $m \to \infty$, and their negative imaginary part tends to 0 exponentially fast as $m \to \infty$. Additionally, a closer observation gives us that $\Re(\ell_m^2) \propto m^2$. Figure 5 represents the behavior of w_8 for the three types of resonances far from the boundary for $a_{\mathsf{c}} \in \{-1.1, -0.9\}$. As discussed above, the support of the inner and outer resonant modes is mainly inside and outside the cavity, respectively. The modes associated to interface resonances are locally exponentially decreasing moving away from the interface, which is the mathematical characterization of surface plasmons [29, 8]. In the next section, we characterize to leading order these interface resonances family $(\ell_m)_{m\geq 1}$ by performing asymptotic expansion as $m \to \infty$. In particular, we will confirm that $\ell_m \propto m$.

Remark 3.5. As seen above, it is convenient to identify the change of behavior of the interface resonances using $\Re(\ell_m^2)$. In what follows we provide asymptotic expansions of $(\ell_m^2)_{m\geq 1}$ instead of the resonances $(\ell_m)_{m\geq 1}$.

Remark 3.6. Going back to the Eq. (2.2), it turns out that the dashed blue line in Fig. 1 corresponds to the real part an interface resonance: $k_8 = \Re(\ell_8) \approx 2.377$, and $\ell_8 \in \mathcal{R}_{\mathsf{pla}}[-1.1, 1]$. Additionally, given data associated to $k > 0$, the interface modes associated to $\ell \in \mathcal{R}_{\mathsf{pla}}[-0.9, 1]$ (in other words $\Re(\ell^2) < 0$) cannot be excited as illustrated in Fig. 1. One can also perform the same computations for a lossy circular cavity. In that case the interface resonances plunge further into the complex plane (their imaginary part gets further away from the real axis). Excitation of those resonances is then more difficult to observe.

3.2. **Interpretation with Schrödinger operator for the disk.** From Section 3.1 we found that plasmonic resonances $(\ell_m)_m$ are such that $\Re(\ell_m^2)$ changes sign depending on a_{c} (*i.e.* η). In this section we use asymptotic expansions to explain this change of behavior at leading order. To do so we provide an analogy with the Schrödinger operator. We define $\check{\lambda} = m^{-2}\,\ell^2$, and we rewrite Problem Eq. (3.7) as

$$\begin{cases} -m^{-2}\dfrac{1}{r}\partial_r\left(r\,\partial_r w_m^{\pm}\right) + \dfrac{1}{r^2}w_m^{\pm} = a(r)\,\check{\lambda} w_m^{\pm} & \text{in } (0,R)\cup(R,+\infty) \\ w_m^-(R) = w_m^+(R) \text{ and } -\eta^{-2}\,\partial_r w_m^-(R) = \partial_r w_m^+(R) & \text{across } \{R\} \\ w_0^{-\prime}(0) = 0 \text{ and } w_m^+ \in \mathscr{S}([R,+\infty)) \end{cases} \tag{3.11}$$

with $\check{\lambda}$ the new spectral parameter, $w_m^{\pm}$ restrictions of w_m in each material, and $\mathscr{S}(\mathbb{R}_+)$ denoting the Schwartz space. We replace the outgoing wave condition by the requirement that w_m^+ belongs to the Schwartz space in order to characterize exponentially decreasing behaviors from both sides of the interface (*i.e.* surface plasmons). To identify this behavior, first we rescale the problem Eq. (3.11) by $\xi = r/R - 1$ such that $r = R$ corresponds to $\xi = 0$. We then define $v_m^{\pm}(\xi) = w_m^{\pm}(R\,(1+\xi))$, satisfying in particular

$$-m^{-2}\,\mathscr{L}v_m^{\pm} + V v_m^{\pm} = a(\xi)\,R^2\check{\lambda}\,v_m^{\pm} \qquad \text{in } (-1,0) \text{ and } (1,+\infty),$$

where $\mathscr{L}(\xi,\partial_\xi) = \frac{1}{1+\xi}\partial_\xi((1+\xi)\,\partial_\xi)$ is a positive elliptic operator (Laplacian like) and $V(\xi) = \frac{1}{(1+\xi)^2}$ is a potential. In that sense, the operator $v \mapsto (-m^{-2}\,\mathscr{L} + V)v$ can be interpreted as a Schrödinger operator. To construct localized modes at the interface, we consider the principal part of $-m^{-2}\mathscr{L} + V$ with its coefficients frozen at $\xi = 0$, corresponding to $-m^{-2}\partial_\xi^2 + 1$. It is then natural to rescale by $\rho = m\xi$, and the leading order behavior becomes

$$\begin{cases} -\partial_\rho^2\varphi^- + \varphi^- = -\eta^2\, R^2\breve{\lambda}\,\varphi^- & \text{in } (-\infty,0) \\ -\partial_\rho^2\varphi^+ + \varphi^+ = R^2\breve{\lambda}\,\varphi^+ & \text{in } (0,+\infty) \\ \varphi^-(0) = \varphi^+(0) \text{ and } \eta^{-2}\,\partial_\rho\varphi^-(0) = \partial_\rho\varphi^+(0) & \text{across } \{0\}, \\ \varphi^\pm \in \mathscr{S}(\mathbb{R}_\pm) \end{cases} \tag{3.12}$$

with $\varphi^\pm(\rho) = v_m^\pm(\xi)$. Note that the condition $v_m^-(-1) = \varphi^-(-m) = 0$ becomes $\varphi^- \in \mathscr{S}(\mathbb{R}_-)$ to keep a localized behavior as $m \to +\infty$. Solutions of Eq. (3.12) are given by $(\breve{\lambda}, \varphi^\pm) = (R^{-2}(1-\eta^{-2}), \mathsf{e}^{-\eta^{\mp 1}|\rho|})$, where the modes are exponentially decreasing on both sides of the interface $\rho = 0$. Back to Eq. (3.11), we have found a pair $(\underline{\lambda}_m, \underline{w}_m^\pm)$ characterizing $(\ell^2, w_m^\pm)$, with the leading behavior given by

$$\underline{\lambda}_m = \frac{m^2}{R^2}\left(1-\eta^{-2}\right) + \mathcal{O}(m^{-1}), \quad \text{and} \quad \underline{w}_m^\pm(r) = \exp\left(-\eta^{\mp 1} m \left|\frac{r}{R} - 1\right|\right) + \mathcal{O}(m^{-1}). \tag{3.13}$$

We conclude:

- when $a_\mathsf{c} < -1$ ($\eta > 1$), surface plasmons waves are associated to scattering resonances with $\Re(\ell^2) > 0$ (at first order);
- when $-1 < a_\mathsf{c} < 0$ ($0 < \eta < 1$), surface plasmons waves are associated to scattering resonances with $\Re(\ell^2) < 0$ (at first order).

We have then asymptotically characterized SPW by building pairs $(\underline{\lambda}_m, \underline{w}_m)_{m\geq 1}$. Upon proper justification that $\underline{w}_m(r)e^{\mathrm{i}m\theta} \in D(P)$ and that $k = \underline{k}_m := \sqrt{(\underline{\lambda}_m)}$ affects the resolvent, the obtained results match the observed behaviors in previous sections, and provide accurate predictions.

The case of the circular cavity with constant a_c is quite intuitive, and the leading order computations can be done explicitly. In the next sections we generalize the approach, to any order, for the general case (arbitrary shaped smooth boundary, and varying coefficients $a_\mathsf{c} \in \mathscr{C}^\infty(\overline{\Omega}; (-\infty,-1)\cup(-1,0))$), and justify the connection between the formal expansions (Section 4) and the resolvent operator (as well as the scattering instabilities, consequently) (Section 5). To that aim, we will use semi-classical WKB (Wentzel-Kramers-Brillouin) expansions along the interface and matched asymptotic expansions in the transverse direction to the interface in a tubular neighborhood of the interface. The higher order terms allow to show a super-algebraic behavior of the peaks seen in Fig. 1, explaining the exponential increase asymptotically.

4. Quasi-pair for unbounded transmission problems with sign-changing coefficient

In this section we prove Theorem 2.3 which consists of constructing approximate solutions of the resonance problem Eq. (2.3). Those solutions are called quasi-pairs, in the sense of Definition 2.2. The proof is organized as follows:

- We define a tubular neighborhood where we set up the problem, and we define formal expansions (Section 4.1).
- We compute the expansion terms by solving a family of problems indexed by the order of the expansions (Section 4.2).
- We show that the obtained expansions are quasi-pairs in the sense of Definition 2.2 (Lemma 4.9), and that the quasi-resonances are independent of the construction (Corollary 4.13). Details are given in Section 4.3.

We end Section 4 with comments on the first expansion terms of $(\underline{\lambda}_m)_{m\geq 1}$.

4.1. **Formal expansion setup.** Recall that $\Omega \subset \mathbb{R}^2$ is a cavity with smooth boundary Γ, see Section 2.1. Let L be the length of Γ, and $\eta := \sqrt{-a_{\mathsf{c}}}$ a positive smooth function up to the interface so that we have $a_{\mathsf{c}} = -\eta^2$. We define a tubular neighborhood $\mathcal{V}_\delta$ of the interface Γ. Let $\gamma\colon \mathbb{T}_L \to \Gamma$ be a counterclockwise curvilinear parametrization of the curve Γ with the notation $\mathbb{T}_L := \mathbb{R}/L\mathbb{Z}$. Let $n = (\gamma_2', -\gamma_1')^\intercal$ be the unit exterior normal to Ω and $\kappa = \det(\gamma', \gamma'') : \mathbb{T}_L \to \mathbb{R}$ be the signed curvature. We define the open tubular neighborhood, see [35], by

$$\mathcal{V}_\delta := \{\gamma(s) + \xi n(s) \mid (s, \xi) \in \mathbb{T}_L \times (-\delta, \delta)\} \tag{4.1}$$

which is schematically represented in Fig. 6.

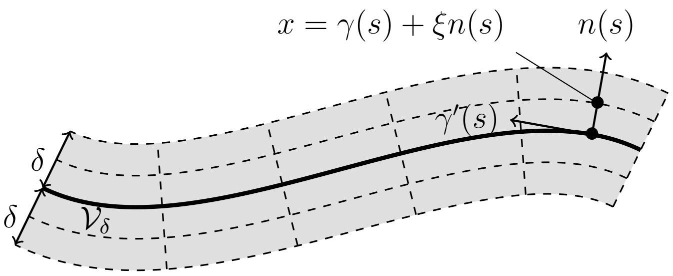


Figure 6. *Tubular neighborhood and notations: s denotes an arc-length parametrization of the curve γ, and ξ is the normal variable.*

We now consider the problem:

$$\begin{cases} Pu = \lambda u & \text{in } \Omega \cap \mathcal{V}_\delta \text{ and } \left(\mathbb{R}^2 \setminus \overline{\Omega}\right) \cap \mathcal{V}_\delta \\ [u]_\Gamma = 0 \text{ and } \left[a^{-1}\,\partial_n u\right]_\Gamma = 0 & \text{across } \Gamma, \\ u = 0 & \text{on } \partial\mathcal{V}_\delta \end{cases} \tag{4.2}$$

where $P = -\operatorname{div}(a^{-1}\,\nabla)$ with a defined in Eq. (2.1). By Definition 2.2, the quasi-pairs are compactly supported therefore the outgoing condition does not play a role in their construction. We replace in particular the outgoing wave condition by a homogeneous Dirichlet boundary condition in order to construct localized quasi-pairs.

The change of variables from the tubular coordinates $(s, \xi) \in \mathbb{T}_L \times (-\delta, \delta)$ to the Cartesian coordinates $x \in \mathcal{V}_\delta$ is a smooth diffeomorphism for $0 < \delta < (\max_{\mathbb{T}_L} |\kappa|)^{-1}$. In this tubular coordinate system the operator P becomes

$$P = -g^{-1}\operatorname{div}_{s,\xi}\left(a^{-1}\,G\,\nabla_{s,\xi}\right) \tag{4.3}$$

where $g(s, \xi) = 1 + \xi\kappa(s) > 0$ and $G(s, \xi) = \begin{pmatrix} g(s,\xi)^{-1} & 0 \\ 0 & g(s,\xi) \end{pmatrix}$.

For the general case we use a WKB (Wentzel-Kramers-Brillouin) framework [5] in order to provide an asymptotic expansion of the spectral parameter as the number of oscillations along the interface Γ, denoted m in Section 3.2, goes to infinity. We introduce a small parameter $h > 0$ (later to be linked to m) and the ansatz for the quasi-pair (λ, u):

$$u(s, \xi) = w(s, \xi)\,\exp\left(\tfrac{\mathsf{i}}{h}\,\theta(s)\right) \quad \text{and} \quad \lambda = h^{-2}\,\check{\lambda} \tag{4.4}$$

where $\frac{1}{h}\theta\colon [0, L] \to \mathbb{C}$ is the fast phase along the interface, $w\colon \mathbb{T}_L \times (-\delta, \delta) \to \mathbb{C}$ is the slow amplitude, and $\check{\lambda} \in \mathbb{C}$ is the spectral parameter. In order for the function u in Eq. (4.4) to be a smooth function in $\mathcal{V}_\delta \setminus \Gamma$, we need to add the constraint that the function $s \mapsto \mathsf{e}^{\frac{\mathsf{i}}{h}\theta(s)} \in \mathscr{C}^\infty(\mathbb{T}_L)$. The phase function is chosen to be complex to simplify the computations, however we can always put the imaginary part into the amplitude w. Following [5], we formally expand the unknowns w, θ, and $\breve{\lambda}$ with respect to h as

$$w(s,\xi) = \sum_{n\geq 0} w_n(s,\xi)\; h^n, \quad \theta(s) = \sum_{n\geq 0} \theta_n(s)\; h^n, \quad \text{and} \quad \breve{\lambda} = \sum_{n\geq 0} \breve{\lambda}_n\; h^n. \tag{4.5}$$

The system Eq. (4.2) with the new unknowns Eq. (4.4) becomes

$$\begin{cases} \mathcal{L}_h[a](w,\theta) = \breve{\lambda}\, w & \text{in } \mathbb{T}_L \times [(-\delta,0)\cup(0,\delta)] \\ [w]_{\mathbb{T}_L\times\{0\}} = 0 \text{ and } \left[a^{-1}\,\partial_\xi w\right]_{\mathbb{T}_L\times\{0\}} = 0 & \text{across } \mathbb{T}_L\times\{0\} \\ w = 0 & \text{on } \mathbb{T}_L\times\{-\delta,\delta\} \end{cases}. \tag{4.6}$$

Above, $\mathcal{L}_h[a](w,\theta) = h^2\,\mathsf{e}^{-\frac{\mathsf{i}}{h}\theta}\,P\left(w\,\mathsf{e}^{\frac{\mathsf{i}}{h}\theta}\right)$, and it can be decomposed as

$$\mathcal{L}_h[a](w,\theta) = \mathcal{L}_h^3[a](w,\theta,\theta) + \mathcal{L}_h^2[a](w,\theta) + \mathcal{L}_h^1[a](w) \tag{4.7}$$

where $\mathcal{L}_h^j[a]$ are j-linear for $j\in\{1,2,3\}$ and

$$\mathcal{L}_h^3[a](w,\theta,\vartheta) = g^{-2}\,a^{-1}\,w\,\partial_s\theta\,\partial_s\vartheta, \tag{4.8a}$$

$$\mathcal{L}_h^2[a](w,\theta) = -h\,\mathsf{i}\left(g^{-2}\,a^{-1}\,\partial_s w\,\partial_s\theta + g^{-1}\,\partial_s\left(g^{-1}\,a^{-1}\,w\,\partial_s\theta\right)\right), \tag{4.8b}$$

$$\mathcal{L}_h^1[a](w) = -h^2\,g^{-1}\,\left(\partial_\xi\left(g\,a^{-1}\,\partial_\xi w\right) + \partial_s\left(g^{-1}\,a^{-1}\,\partial_s w\right)\right). \tag{4.8c}$$

In the above decomposition, only $\mathcal{L}_h^1[a]$ involves derivatives with respect to ξ. Since g (resp. $\eta = \sqrt{-a_{\mathsf{c}}} > 0$) is a smooth function on $\mathbb{T}_L\times(-\delta,\delta)$ (resp. $\mathbb{T}_L\times(-\delta,0]$), then G is smooth, and we write the formal Taylor expansions at $\xi=0$:

$$g(s,\xi) = 1+\xi\kappa(s), \quad G(s,\xi) = \sum_{n\geq 0}\frac{\partial_\xi^n G(s,0)}{n!}\,\xi^n, \quad \eta(s,\xi) = \sum_{n\geq 0}\frac{\eta_n(s)}{n!}\,\xi^n, \tag{4.9}$$

where $\eta_n(s) = \partial_\xi^n\eta(s,0)$. Since g and η do not vanish on $\mathbb{T}_L\times\{0\}$, the formal expansions of g^{-1}, g^{-2}, and η^{-2} about $\xi=0$ can be computed with Eq. (4.9).

Like in Section 3.2, we introduce the scaled variable $\rho = h^{-1}\xi$ for the normal variable $\xi\in(-\delta,\delta)$, and we define

$$\varphi^\pm(s,\rho) = w(s,h\rho), \qquad \text{for } (s,\rho)\in\mathbb{T}_L\times\mathbb{R}_\pm.$$

Then, with $g = g(s,h\rho)$ we rewrite

$$\mathcal{L}_h^1[a](\varphi^\pm) = -g^{-1}\,\partial_\rho\left(a^{-1}\,g\,\partial_\rho\varphi^\pm\right) - h^2\,g^{-1}\,\partial_s\left(a^{-1}\,g^{-1}\,\partial_s\varphi^\pm\right). \tag{4.10}$$

Problem Eq. (4.6) becomes the formal problem: Find $(\varphi_n^\pm)_{n\in\mathbb{N}} \in \mathscr{C}^\infty(\mathbb{T}_L,\mathscr{S}(\mathbb{R}_\pm))^{\mathbb{N}}$, $\left(\exp(\tfrac{\mathsf{i}}{h}\theta_n)\right)_{n\in\mathbb{N}} \in \mathscr{C}^\infty(\mathbb{T}_L)^{\mathbb{N}}$, and $(\breve{\lambda}_n)_{n\in\mathbb{N}}\in\mathbb{C}^{\mathbb{N}}$ such that

$$\begin{cases} \mathcal{L}_h[a]\left(\sum_n \varphi_n^\pm\,h^n, \sum_n\theta_n\,h^n\right) = \left(\sum_n\breve{\lambda}_n\,h^n\right)\left(\sum_n\varphi_n^\pm\,h^n\right) & \text{in } \mathbb{T}_L\times\mathbb{R}_\pm^* \\ \sum_n\varphi_n^-(s,0)\,h^n = \sum_n\varphi_n^+(s,0)\,h^n & \text{on } \mathbb{T}_L\times\{0\} \\ -\eta_0(s)^{-2}\sum_n\partial_\rho\varphi_n^-(s,0)\,h^n = \sum_n\partial_\rho\varphi_n^+(s,0)\,h^n & \text{on } \mathbb{T}_L\times\{0\} \end{cases}. \tag{4.11}$$

Note that for simplicity we extend the scaled domain $\mathbb{T}_L\times(-\frac{\delta}{h},\frac{\delta}{h})$ to the domain $\mathbb{T}_L\times\mathbb{R}$ in order to be independent of h in Eq. (4.11), and we replace the homogeneous Dirichlet boundary condition on $\mathbb{T}_L\times\{-\frac{\delta}{h},\frac{\delta}{h}\}$ by the conditions $\rho\mapsto\varphi^\pm(s,\rho)\in\mathscr{S}(\mathbb{R}_\pm)$ for all $s\in\mathbb{T}_L$. One can always multiply the quasi-mode by a cutoff function $\xi\mapsto\chi(\xi)$ to be in the domain $\mathbb{T}_L\times(-\frac{\delta}{h},\frac{\delta}{h})$, as done later in Eq. (4.16). With Eq. (4.7) and Eq. (4.9), we can formally expand the operators $\mathcal{L}_h^j[-\eta^2] = \sum_{n\geq 0}\mathsf{L}_n^{j,-}\,h^n$ and $\mathcal{L}_h^j[1] = \sum_{n\geq 0}\mathsf{L}_n^{j,+}\,h^n$

where $\mathsf{L}_n^{j,\pm}$ are independent of h, for $j \in \{1,2,3\}$. From Problem Eq. (4.11) we obtain the family of problems $(\mathcal{P}_n)_{n\in\mathbb{N}}$ by identifying powers of h: Find $\varphi_n^\pm \in \mathscr{C}^\infty(\mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$, $\exp(\frac{\mathrm{i}}{h}\theta_n) \in \mathscr{C}^\infty(\mathbb{T}_L)$, and $\check{\lambda}_n \in \mathbb{C}$ such that

$$\begin{cases} \displaystyle\sum_{p\in\mathbb{N}_n^4} \mathsf{L}_{p_1}^{3,\pm}\left(\varphi_{p_2}^\pm, \theta_{p_3}, \theta_{p_4}\right) + \sum_{p\in\mathbb{N}_n^3} \mathsf{L}_{p_1}^{2,\pm}\left(\varphi_{p_2}^\pm, \theta_{p_3}\right) + \sum_{p\in\mathbb{N}_n^2} \mathsf{L}_{p_1}^{1,\pm}\left(\varphi_{p_2}^\pm\right) = \sum_{p\in\mathbb{N}_n^2} \check{\lambda}_{p_1}\,\varphi_{p_2}^\pm \\ \varphi_n^-(s,0) = \varphi_n^+(s,0) \quad \text{and} \quad -\eta_0(s)^{-2}\,\partial_\rho\varphi_n^-(s,0) = \partial_\rho\varphi_n^+(s,0) \end{cases} \tag{4.12}$$

with the notation $\mathbb{N}_n^d = \{p \in \mathbb{N}^d \mid p_1 + \cdots + p_d = n\}$.

4.2. **Computation of the expansion terms.** First, we set some notation that will be useful through out the rest of the section.

Notation 4.1. We recall that $\eta_0 = \eta|_\Gamma = \sqrt{-\,a_\mathsf{c}|_\Gamma}$. Since we assume that $1 + a_\mathsf{c}|_\Gamma^{-1} = 1 - \eta_0^{-2} \neq 0$, we can define the scalar $\varsigma = \pm 1$ to be the sign of $1 - \eta_0^{-2}$, the functions $\tau_0 = \left|1 - \eta_0^{-2}\right|^{-\frac{1}{2}}$, and $\widehat{\tau}_0 = \frac{\tau_0}{\langle\tau_0\rangle}$ where $\langle\cdot\rangle$ is the mean along the interface Γ define by

$$\langle f\rangle \coloneqq \frac{1}{L}\int_{\mathbb{T}_L} f(s)\,\mathrm{d}s, \qquad \forall f \in \mathrm{L}^1(\mathbb{T}_L).$$

One can obtain the expressions for the $\mathsf{L}_0^{j,\pm}$.

Lemma 4.2. *The first terms of the expansions of $\mathcal{L}_h^3[a]$, $\mathcal{L}_h^2[a]$, and $\mathcal{L}_h^1[a]$, are given by*

$$\mathsf{L}_0^{3,-}(\phi,\theta,\vartheta) = -\eta_0^{-2}\,\phi\,\partial_s\theta\,\partial_s\vartheta, \qquad \mathsf{L}_0^{2,-}(\phi,\theta) = 0, \qquad \mathsf{L}_0^{1,-}(\phi) = \eta_0^{-2}\,\partial_\rho^2\phi,$$
$$\mathsf{L}_0^{3,+}(\phi,\theta,\vartheta) = \phi\,\partial_s\theta\,\partial_s\vartheta, \qquad \mathsf{L}_0^{2,+}(\phi,\theta) = 0, \qquad \mathsf{L}_0^{1,+}(\phi) = -\partial_\rho^2\phi.$$

Proof. From the expressions (4.8a), (4.8b), and (4.10) and using the expansions (4.9) with the change of variable $\xi = h\rho$ gives the expressions in the lemma. ☐

Using Lemma 4.2, we rewrite Problem $(\mathcal{P}_0)$ as: Find $\varphi_0^\pm \in \mathscr{C}^\infty(\mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$, $\theta_0 \in \mathscr{C}^\infty([0,L])$, and $\check{\lambda}_0 \in \mathbb{C}$ such that $(\varphi_0^-, \varphi_0^+) \not\equiv (0,0)$, $\exp(\frac{\mathrm{i}}{h}\theta_0) \in \mathscr{C}^\infty(\mathbb{T}_L)$, and

$$\begin{cases} \partial_\rho^2\varphi_0^- - \left({\theta_0'}^2 + \eta_0^2\,\check{\lambda}_0\right)\varphi_0^- = 0 & \text{in } \mathbb{T}_L \times \mathbb{R}_- \\ \partial_\rho^2\varphi_0^+ - \left({\theta_0'}^2 - \check{\lambda}_0\right)\varphi_0^+ = 0 & \text{in } \mathbb{T}_L \times \mathbb{R}_+ \\ \varphi_0^-(s,0) = \varphi_0^+(s,0) & \text{on } \mathbb{T}_L \times \{0\} \\ -\eta_0(s)^{-2}\,\partial_\rho\varphi_0^-(s,0) = \partial_\rho\varphi_0^+(s,0) & \text{on } \mathbb{T}_L \times \{0\} \end{cases}. \tag{4.13}$$

Lemma 4.3. *One can choose $h = \frac{L}{2\pi m}$ for $m \in \mathbb{N}^*$ so that $(\varphi_0^\pm, \theta_0, \check{\lambda}_0)$ is given by*

$$\check{\lambda}_0 = \frac{\varsigma}{\langle\tau_0\rangle^2}, \qquad \theta_0(s) = \int_0^s \widehat{\tau}_0(t)\,\mathrm{d}t, \qquad \text{and} \qquad \varphi_0^\pm(s,\rho) = \alpha(s)\exp\left(-|\rho|\,\widehat{\tau}_0(s)\,\eta_0(s)^{\mp 1}\right),$$

with $\alpha \in \mathscr{C}^\infty(\mathbb{T}_L, \mathbb{C}^*)$, is solution of Problem $(\mathcal{P}_0)$ defined in Eq. (4.13).

The proof is detailed in Appendix B.1.

Remark 4.4. • If we unravel the scaling and return to tubular coordinates, for $m \geq 1$ and $(s,\xi) \in \mathbb{T}_L \times \mathbb{R}$, we formally have a pair $(\underline{\lambda}_m, \underline{u}_m)$

$$\underline{\lambda}_m = \left(\frac{2\pi m}{L}\right)^2\left[\check{\lambda}_0 + \mathcal{O}\left(m^{-1}\right)\right],$$

$$\underline{u}_m(s,\xi) = \mathrm{e}^{\mathrm{i}\frac{2\pi m}{L}\left[\theta_0(s) + \mathcal{O}\left(m^{-1}\right)\right]}\begin{cases} \varphi_0^-\left(s, \frac{2\pi m}{L}\xi\right) & \text{if } \xi \leq 0 \\ \varphi_0^+\left(s, \frac{2\pi m}{L}\xi\right) & \text{if } \xi > 0 \end{cases} + \mathcal{O}\left(m^{-1}\right),$$

which characterizes surface plasmons at leading order.

- We remark that the leading order term, solution of Eq. (4.13), can be seen as the leading order solution of a planar problem of the form $-\operatorname{div}(a^{-1}\nabla v) = \nu v$ on $\mathbb{T}_L \times \mathbb{R}$ with $a(s,y) = -\eta_0^2$ on the lower half-plane, $a \equiv 1$ on the upper half-plane, and $\nu \in \mathbb{R}$.

Remark 4.5. The construction relies on several choices that are not unique.

- One can choose the main phase to satisfy $\theta_0' = \widehat{\tau}_0$ or $\theta_0' = -\widehat{\tau}_0$. Then one can construct two modes corresponding to $\underline{u}_m$ and $\overline{\underline{u}_m}$ (see Remark 4.14), where $\overline{\cdot}$ is the complex conjugate.
- The function θ_0 is defined up to a constant c. Then $\underline{u}_m$ in Remark 4.4 is defined up to $\mathrm{e}^{\mathrm{i}\frac{2\pi m}{L}c}$. For simplicity, we consider $c = 0$ as we normalize in the end.
- The functions $\varphi_0^\pm$ are defined up to a function $\alpha : \mathbb{T}_L \to \mathbb{C}^*$, which contributes to the phase of $\underline{u}_m$ and therefore affects the number of oscillations along the interface. One can always shift indices so that $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1-q_\alpha}$, for some $q_\alpha \in \mathbb{Z}$, corresponds to a wave with m oscillations along the interface.
- We choose $h = \frac{L}{2\pi m}$ to simplify the computations however other choices can be made, as long as we have $h \propto m^{-1}$.

Now, to compute the higher order term of the expansion, from Eq. (4.12), Lemma 4.2, and Lemma 4.3, for $n \geq 1$, we can rewrite Problem $(\mathcal{P}_n)$ as: Find $\varphi_n^\pm \in \mathscr{C}^\infty(\mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$, $\exp(\mathrm{i}\, h^{n-1}\,\theta_n) \in \mathscr{C}^\infty(\mathbb{T}_L)$, and $\check{\lambda}_n \in \mathbb{C}$ such that

$$\begin{cases} \partial_\rho^2 \varphi_n^- - \widehat{\tau}_0^2\, \eta_0^2\, \varphi_n^- = \left(2\widehat{\tau}_0\, \theta_n' + \eta_0^2\, \check{\lambda}_n\right) \varphi_0^- + \eta_0^2\, S_{n-1}^- & \text{in } \mathbb{T}_L \times \mathbb{R}_- \\ \partial_\rho^2 \varphi_n^+ - \widehat{\tau}_0^2\, \eta_0^{-2}\, \varphi_n^+ = \left(2\widehat{\tau}_0\, \theta_n' - \check{\lambda}_n\right) \varphi_0^+ - S_{n-1}^+ & \text{in } \mathbb{T}_L \times \mathbb{R}_+ \\ \varphi_n^-(s,0) = \varphi_n^+(s,0) & \text{on } \mathbb{T}_L \times \{0\}, \\ -\eta_0(s)^{-2}\, \partial_\rho \varphi_n^-(s,0) = \partial_\rho \varphi_n^+(s,0) & \text{on } \mathbb{T}_L \times \{0\} \end{cases} \tag{4.14}$$

where

$$\begin{aligned} S_{n-1}^\pm = \sum_{p=1}^{n-1} \check{\lambda}_{n-p}\, \varphi_p^\pm - \sum_{p=0}^{n-1} \mathsf{L}_{n-p}^{1,\pm}\left(\varphi_p^\pm\right) - \sum_{p\in\mathbb{I}_n^3} \mathsf{L}_{p_1}^{2,\pm}\left(\varphi_{p_2}^\pm, \theta_{p_3}\right) \\ - \mathsf{L}_n^{2,\pm}\left(\varphi_0^\pm, \theta_0\right) - \sum_{p\in\mathbb{I}_n^4} \mathsf{L}_{p_1}^{3,\pm}\left(\varphi_{p_2}^\pm, \theta_{p_3}, \theta_{p_4}\right) - \mathsf{L}_n^{3,\pm}\left(\varphi_0^\pm, \theta_0, \theta_0\right) \end{aligned} \tag{4.15}$$

with $\mathbb{I}_n^d = \left\{p \in [\![0, n-1]\!]^d \;\middle|\; p_1 + \cdots + p_d = n\right\}$.

Lemma 4.6. *Define $(\varphi_0^\pm, \theta_0, \check{\lambda}_0)$ according to Lemma 4.3. For $n \geq 1$, there exists a solution $(\varphi_n^\pm, \theta_n, \check{\lambda}_n) \in \mathscr{C}^\infty(\mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm)) \times \mathscr{C}^\infty(\mathbb{T}_L) \times \mathbb{C}$ of Problem $(\mathcal{P}_n)$ defined in Eq. (4.14). In particular, $\varphi_n^\pm$ is given by*

$$\varphi_n^\pm(s,\rho) = P_n^\pm(s,\rho) \exp\left(-|\rho|\, \widehat{\tau}_0(s)\, \eta_0(s)^{\mp 1}\right),$$

with polynomials $P_n^\pm \in \mathscr{C}^\infty(\mathbb{T}_L, \mathbb{P})$[3].

The proof is detailed in Appendix B.2.

Remark 4.7. In addition to Remark 4.5, $(\theta_n)_{n\geq 0}$ and $(\varphi_n)_{n\geq 0}$ are not uniquely defined at each step of the construction. However, the sequence $(\check{\lambda}_n)_{n\geq 0}$ will be unique (see Corollary 4.13).

[3]We denote $\mathbb{P}$ the space of polynomial of a single variable with complex coefficients.

4.3. **Proof of the Theorem 2.3.** Based on formal series $\sum_n \varphi_n^\pm h^n$, $\sum_n \theta_n h^n$, and $\sum_n \breve{\lambda}_n h^n$ with $h = \frac{L}{2\pi m}$, we now construct quasi-pairs in the sense of Definition 2.2. This step is necessary to justify that our formal expansions capture scattering resonances. First we use Borel's Lemma [27, Thm. 1.2.6] for $\breve{\lambda}$ and θ, and a direct generalization on the Fréchet space $\mathscr{C}^\infty(\mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$ [6, Lem. A.5] for $\varphi^\pm$ to establish:

Lemma 4.8. *There exist* $\Phi^\pm \in \mathscr{C}^\infty([0, \frac{L}{2\pi}] \times \mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$, $\Theta \in \mathscr{C}^\infty([0, \frac{L}{2\pi}] \times \mathbb{T}_L)$, *and* $\Lambda \in \mathscr{C}^\infty([0, \frac{L}{2\pi}])$ *such that, for* $N \geq 1$, $h \in [0, \frac{L}{2\pi}]$, $s \in \mathbb{T}_L$, *and* $\rho \in \mathbb{R}_\pm$, *we have*

$$\Phi^\pm(h; s, \rho) = \sum_{n=0}^{N-1} \varphi_n^\pm(s, \rho)\, h^n + h^N\, R_N^\pm(h; s, \rho)$$

$$\Theta(h; s) = \sum_{n=0}^{N-1} \theta_n(s)\, h^n + h^N\, R_N^\Theta(h; s)$$

$$\Lambda(h) = \sum_{n=0}^{N-1} \breve{\lambda}_n\, h^n + h^N\, R_N^\Lambda(h)$$

where $R_N^\pm \in \mathscr{C}^\infty([0, \frac{L}{2\pi}] \times \mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$, $R_N^\Theta \in \mathscr{C}^\infty([0, \frac{L}{2\pi}] \times \mathbb{T}_L)$, $R_N^\Lambda \in \mathscr{C}^\infty([0, \frac{L}{2\pi}])$.

From those functions, we now define the scalars $\underline{\lambda}_m$ and the functions $\underline{u}_m$ in the tubular neighborhood as

$$\underline{\lambda}_m = \left(\tfrac{2\pi m}{L}\right)^2 \Lambda\left(\tfrac{L}{2\pi m}\right) = \left(\tfrac{2\pi m}{L}\right)^2 \sum_{n\in\mathbb{N}} \breve{\lambda}_n \left(\tfrac{2\pi m}{L}\right)^n \tag{4.16a}$$

$$\underline{u}_m(s, \xi) = \chi(\xi) \exp\left(\mathrm{i}\tfrac{2\pi m}{L}\, \Theta\left(\tfrac{L}{2\pi m}; s\right)\right) \begin{cases} \Phi^-\left(\tfrac{L}{2\pi m}; s, \tfrac{2\pi m}{L}\xi\right) & \text{if } \xi \leq 0 \\ \Phi^+\left(\tfrac{L}{2\pi m}; s, \tfrac{2\pi m}{L}\xi\right) & \text{if } \xi > 0 \end{cases}, \tag{4.16b}$$

where χ is a cutoff function, $\chi \in \mathscr{C}^\infty_{\mathrm{comp}}((-\delta, \delta))$ and $\chi \equiv 1$ on $\left[-\frac{\delta}{2}, \frac{\delta}{2}\right]$. In what follows, we establish that Eq. (4.16) is a quasi-pair. First we have:

Lemma 4.9. *The pair* $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$ *defined in* Eq. (4.16) *satisfies the following:*

(i) $\underline{u}_m$ *is uniformly compactly supported and smooth in* Ω *and* $\mathbb{R}^2 \setminus \overline{\Omega}$.
(ii) $\underline{u}_m$ *satisfies* $[\underline{u}_m]_\Gamma = \mathcal{O}\left(m^{-\infty}\right)$ *and* $[a^{-1}\, \partial_n \underline{u}_m]_\Gamma = \mathcal{O}\left(m^{-\infty}\right)$.
(iii) $\underline{u}_m$ *admits the norm expansion*

$$\|\underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = b\, m^{-\frac{1}{2}} + \mathcal{O}(m^{-\frac{3}{2}}) \qquad \text{with } b > 0.$$

(iv) Let $\underline{R}_m := P\underline{u}_m - \underline{\lambda}_m\, \underline{u}_m$ *be the reminder defined in* Ω *and* $\mathbb{R}^2 \setminus \overline{\Omega}$, *then we have*

$$\|\underline{R}_m\|_{\mathrm{L}^2(\Omega)} + \|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2\setminus\overline{\Omega})} = \mathcal{O}\left(m^{-\infty}\right).$$

(v) If two quasi-pairs $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$, $(\underline{\mu}_m, \underline{v}_m)_{m\geq 1}$ *satisfy (i)–(iv), and the quasi-modes have the same leading phase* $\theta_0(s) = \int_0^s \widehat{\tau}_0(t)\, \mathrm{d}t$ *then:*

$$\int_{\mathbb{R}^2} \underline{u}_m\, \overline{\underline{v}_m}\, \mathrm{d}x = z_0\, m^{-1} + \mathcal{O}(m^{-2}) \quad \text{and} \quad \int_{\mathbb{R}^2} \underline{u}_m\, \underline{v}_m\, \mathrm{d}x = \mathcal{O}(m^{-\infty})$$

with $z_0 \in \mathbb{C}^*$.

Remark 4.10. Items *(iii)* and *(v)* of Lemma 4.9 give us

$$\int_{\mathbb{R}^2} \frac{\underline{u}_m}{\|\underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)}}\, \frac{\overline{\underline{v}_m}}{\|\overline{\underline{v}_m}\|_{\mathrm{L}^2(\mathbb{R}^2)}}\, \mathrm{d}x = z_0' + \mathcal{O}(m^{-1}), \quad \text{with } z_0' \in \mathbb{C}^*.$$

Remark 4.11. At this point $\underline{u}_m \notin \mathcal{D}(P)$ because the transmission conditions are not exactly satisfied, therefore it is not yet a quasi-pair in the sense of Definition 2.2.

Proof of Lemma 4.9. Recall that we set $h = \frac{L}{2\pi m}$, and to simplify notations we denote $\chi_h : \rho \mapsto \chi(\rho h)$, $\Phi_h^\pm : (s,\rho) \mapsto \Phi^\pm(h;s,\rho)$, $\Theta_h : s \mapsto \Theta(h;s)$, and $\Lambda_h = \Lambda(h)$.

(i) By definition of $(\underline{u}_m)_{m\geq 1}$ in Eq. (4.16b), *(i)* is satisfied.

(ii) Using Lemma 4.8 and that each functions $\varphi_n^\pm$ satisfies the transmission conditions via Lemma 4.6, one can show that $[\underline{u}_m]_\Gamma = \mathcal{O}(m^{-N})$ and $[a^{-1}\,\partial_n \underline{u}_m]_\Gamma = \mathcal{O}(m^{-N})$ for all $N \geq 0$, which is the definition of $\mathcal{O}(m^{-\infty})$.

(iii) We introduce the weighted L^2 semi-norm on $\mathbb{T}_L \times \mathbb{R}_\pm$

$$\|f\|^2_{\mathrm{L}^2_\pm[h]} = \int_{\mathbb{T}_L} \int_{\mathbb{R}_\pm \cap (-\frac{\delta}{h},\frac{\delta}{h})} |f(s,\rho)|^2 \; h(1+\kappa(s)\rho h)\,\mathrm{d}\rho\,\mathrm{d}s. \tag{4.17}$$

Form Eq. (4.16), we obtain

$$\|\underline{u}_m\|^2_{\mathrm{L}^2(\mathbb{R}^2)} = \left\|\chi_h \Phi_h^- \mathrm{e}^{\frac{\mathrm{i}}{h}\Theta_h}\right\|^2_{\mathrm{L}^2_-[h]} + \left\|\chi_h \Phi_h^+ \mathrm{e}^{\frac{\mathrm{i}}{h}\Theta_h}\right\|^2_{\mathrm{L}^2_+[h]}.$$

From Lemma 4.3 and Lemma 4.8 for $N = 1$, we have

$$\Theta_h(s) = \int_0^s \widehat{\tau}_0(t)\,\mathrm{d}t + \theta_1(s) h + h^2\, R_2^\Theta(h;s)$$
$$\Phi_h^\pm(s,\rho) = \alpha(s)\,\exp\left(-|\rho|\,\widehat{\tau}_0(s)\,\eta_0(s)^{\mp 1}\right) + h\,R_1^\pm(h;s,\rho)$$

where $R_2^\Theta \in \mathscr{C}^\infty([0,\frac{L}{2\pi}] \times \mathbb{T}_L)$ and $R_1^\pm \in \mathscr{C}^\infty([0,\frac{L}{2\pi}] \times \mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$. We deduce that

$$\left| \left\|\chi_h \Phi_h^\pm \mathrm{e}^{\frac{\mathrm{i}}{h}\Theta_h}\right\|^2_{\mathrm{L}^2_\pm[h]} - \left\|\chi_h\,\alpha\,\mathrm{e}^{-|\rho|\,\widehat{\tau}_0\eta_0^{\mp1}}\,\mathrm{e}^{\mathrm{i}\,\theta_1}\right\|^2_{\mathrm{L}^2_\pm[h]} \right| \leq C_1^\pm h^2$$

for $C_1^\pm$ some positive constant. We write $\left\|\chi_h\,\alpha\,\mathrm{e}^{-|\rho|\,\widehat{\tau}_0\eta_0^{\mp1}}\,\mathrm{e}^{\mathrm{i}\,\theta_1}\right\|^2_{\mathrm{L}^2_\pm[h]} = I_1^\pm + I_2^\pm + I_3^\pm$,

$$I_1^\pm = h\int_{\mathbb{T}_L}\int_{\mathbb{R}_\pm} |\alpha(s)|^2 \mathrm{e}^{\mp 2\rho\,\widehat{\tau}_0(s)\eta_0(s)^{\mp1}}\,\mathrm{e}^{-2\Im\theta_1(s)}\,\mathrm{d}\rho\,\mathrm{d}s = h\int_{\mathbb{T}_L} \frac{|\alpha(s)|^2\mathrm{e}^{-2\Im\theta_1(s)}}{2\widehat{\tau}_0(s)\eta_0(s)^{\mp1}}\,\mathrm{d}s,$$
$$I_2^\pm = h\int_{\mathbb{T}_L}\int_{\mathbb{R}_\pm} (|\chi(\rho h)|^2 - 1)|\alpha(s)|^2 \mathrm{e}^{\mp 2\rho\,\widehat{\tau}_0(s)\eta_0(s)^{\mp1}}\,\mathrm{e}^{-2\Im\theta_1(s)}\,\mathrm{d}\rho\,\mathrm{d}s,$$
$$I_3^\pm = h^2\int_{\mathbb{T}_L}\int_{\mathbb{R}_\pm} |\chi(\rho h)\alpha(s)|^2 \mathrm{e}^{\mp 2\rho\,\widehat{\tau}_0(s)\eta_0(s)^{\mp1}}\,\mathrm{e}^{-2\Im\theta_1(s)}\,\kappa(s)\rho\,\mathrm{d}\rho\,\mathrm{d}s.$$

One can show that $I_2^\pm = \mathcal{O}(h^\infty)$ using Lemma B.1. Since χ is bounded and the function $(h;s,\rho) \mapsto |\alpha|^2\mathrm{e}^{\mp 2\rho\,\widehat{\tau}_0\eta_0^{\mp1}}\mathrm{e}^{-2\Im\theta_1}\kappa\rho$ is in $\mathscr{C}^\infty([0,\frac{L}{2\pi}] \times \mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$ there exists a constant $C_3^\pm$ such that $|I_3^\pm| \leq C_3^\pm h^2$. Combining the results we get

$$\|\underline{u}_m\|^2_{\mathrm{L}^2(\mathbb{R}^2)} = b^2\, m^{-1} + \mathcal{O}(m^{-2})$$

with

$$b^2 = \frac{L}{2\pi}\frac{I_1^+ + I_1^-}{h} = \frac{L}{2\pi}\int_{\mathbb{T}_L} |\alpha(s)|^2\,\mathrm{e}^{-2\Im(\theta_1(s))}\,\frac{\eta_0(s)^{-1} + \eta_0(s)}{2\widehat{\tau}_0(s)}\,\mathrm{d}s > 0.$$

(iv) Revisiting the change of variables in tubular coordinates and the scaling, we get

$$\|\underline{R}_m\|_{\mathrm{L}^2(\Omega)} = h^{-2}\left\|\mathrm{e}^{\mathrm{i}\,h^{-1}\Theta_h}\left(\mathcal{L}_h[a](\,\cdot\,,\Theta_h) - \Lambda_h\right)\left(\chi_h\,\Phi_h^-\right)\right\|_{\mathrm{L}^2_-[h]}, \tag{4.18a}$$

$$\|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2\setminus\overline{\Omega})} = h^{-2}\left\|\mathrm{e}^{\mathrm{i}\,h^{-1}\Theta_h}\left(\mathcal{L}_h[a](\,\cdot\,,\Theta_h) - \Lambda_h\right)\left(\chi_h\,\Phi_h^+\right)\right\|_{\mathrm{L}^2_+[h]} \tag{4.18b}$$

with $\mathcal{L}_h[a]$ defined in Eq. (4.6). Lemma 4.8 with $N = 1$ and Lemma 4.3 give the estimation $\Im\Theta_h = \mathcal{O}(h)$, so there exists $c_\Theta > 0$ such that $|\mathrm{e}^{\mathrm{i}\,h^{-1}\Theta_h}| \leq c_\Theta$. Introducing the commutator $[\mathcal{L}_h[a](\,\cdot, \Theta_h), \chi_h]$ of the differential operator $\Phi \mapsto \mathcal{L}_h[a](\Phi, \Theta_h)$ with the scaled cutoff function χ_h, we deduce from Eq. (4.18)

$$\|\underline{R}_m\|_{\mathrm{L}^2(\Omega)} \leq c_\Theta\, h^{-2} \left(\mathcal{N}_- + \mathcal{N}_-'\right) \quad \text{and} \quad \|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2\setminus\overline{\Omega})} \leq c_\Theta\, h^{-2} \left(\mathcal{N}_+ + \mathcal{N}_+'\right) \tag{4.19}$$

where $\mathcal{N}_\pm = \left\|\chi_h\big(\mathcal{L}_h[a](\,\cdot, \Theta_h) - \Lambda_h\big)\, \Phi_h^\pm\right\|_{\mathrm{L}^2_\pm[h]}$ and $\mathcal{N}_\pm' = \left\|[\mathcal{L}_h[a](\,\cdot, \Theta_h), \chi_h]\, \Phi_h^\pm\right\|_{\mathrm{L}^2_\pm[h]}$. Let's start with $\mathcal{N}_\pm$. We write for $N \geq 1$,

$$\mathcal{L}_h[a](\Phi_h^\pm, \Theta_h) = \sum_{n=0}^{N-1} h^n \left(\mathbf{L}_n^{\pm,3}(\Phi_h^\pm, \Theta_h, \Theta_h) + \mathbf{L}_n^{\pm,2}(\Phi_h^\pm, \Theta_h) + \mathbf{L}_n^{\pm,1}(\Phi_h^\pm)\right)$$
$$+ h^N \left(\mathbf{R}_N^{\pm,3}(h; \Phi_h^\pm, \Theta_h, \Theta_h) + \mathbf{R}_N^{\pm,2}(h; \Phi_h^\pm, \Theta_h) + \mathbf{R}_N^{\pm,1}(h; \Phi_h^\pm)\right)$$

where $\mathbf{R}_N^{\pm,j}(h)$ are j-linear second order differential operators such that all the coefficients in $\chi_h\, \mathbf{R}_N^{\pm,j}(h)$ are smooth bounded functions for $j \in \{1, 2, 3\}$. We use Lemma 4.8 with different N for each occurrence of $\Phi_h^\pm$ and Θ_h, and we obtain

$$\begin{aligned}
&\mathcal{L}_h[a](\Phi_h^\pm, \Theta_h) - \Lambda_h \Phi_h^\pm \\
&= h^N \Bigg[\sum_{n=0}^{N-1} \sum_{p \in \mathbb{N}^3_{N-n}} \mathbf{L}_n^{\pm,3}(R_{p_1}^\pm(h), R_{p_2}^\Theta(h), R_{p_3}^\Theta(h)) + \mathbf{R}_N^{\pm,3}(h; R_0^\pm(h), R_0^\Theta(h), R_0^\Theta(h)) \\
&\quad + \sum_{n=0}^{N-1} \sum_{p \in \mathbb{N}^2_{N-n}} \mathbf{L}_n^{\pm,2}(R_{p_1}^\pm(h), R_{p_2}^\Theta(h)) + \mathbf{R}_N^{\pm,2}(h; R_0^\pm(h), R_0^\Theta(h)) \\
&\quad + \sum_{n=0}^{N-1} \left(\mathbf{L}_n^{\pm,1} - \breve{\lambda}_n\right) R_{N-n}^\pm(h) + \mathbf{R}_N^{\pm,1}(h; R_0^\pm(h)) - R_N^\Lambda(h) R_0^\pm(h)\Bigg]
\end{aligned} \tag{4.20}$$

where we used the relations in Eq. (4.12), giving us that for all $Q \in \mathbb{N}$

$$\sum_{p \in \mathbb{N}^4_Q} \mathbf{L}_{p_1}^{3,\pm} \left(\varphi_{p_2}^\pm, \theta_{p_3}, \theta_{p_4}\right) + \sum_{p \in \mathbb{N}^3_Q} \mathbf{L}_{p_1}^{2,\pm} \left(\varphi_{p_2}^\pm, \theta_{p_3}\right) + \sum_{p \in \mathbb{N}^2_Q} \left(\mathbf{L}_{p_1}^{1,\pm} - \breve{\lambda}_{p_1}\right) \varphi_{p_2}^\pm = 0.$$

The coefficients in the operator $\chi_h \mathcal{L}_h[a](\,\cdot, \Theta_h)$ are smooth bounded functions in $\mathbb{T}_L \times \mathbb{R}_\pm$ (see Eqs. (4.10), (4.8a) and (4.8b)). From Eq. (4.20), we get $\mathcal{N}_\pm \leq h^N\, \|F^\pm(h)\|_{\mathrm{L}_\pm[h]}$ where $F^\pm \in \mathscr{C}^\infty([0, \frac{L}{2\pi}] \times \mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$, so we have $\mathcal{N}_\pm \leq C_N\, h^N$ for C_N a constant independent of h as $h \to 0$. Now, we consider the two commutator norms $\mathcal{N}_\pm'$. We observe that the coefficients of the operators $[\mathcal{L}_h[a](\,\cdot, \Theta_h), \chi_h]$ are zero in $\mathbb{T}_L \times (-\frac{\delta}{2h}, 0)$ and $\mathbb{T}_L \times (0, \frac{\delta}{2h})$. From this observation, we deduce that

$$\mathcal{N}_\pm'^{\,2} = \int_{\mathbb{T}_L} \int_{I_\pm(h)} |G^\pm(h; s, \rho)|^2 \,\mathrm{d}\rho \,\mathrm{d}s$$

where $G^\pm \in \mathscr{C}^\infty([0, \frac{L}{2\pi}] \times \mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$ and $I_\pm(h)$ are as in Lemma B.1 for $\rho = \frac{\delta}{2}$. We deduce that $\mathcal{N}_\pm' = \mathcal{O}(h^\infty)$, and we get $\|\underline{R}_m\|_{\mathrm{L}^2(\Omega)} + \|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2\setminus\overline{\Omega})} = \mathcal{O}\left(h^{N-2}\right)$ for all $N > 1$.

(v) Let $(\theta_n)_{n\geq 0}$ (resp. $(\vartheta_n)_{n\geq 0}$) be a sequence of phases constructed for $\underline{u}_m$ (resp. $\underline{v}_m$) and α (resp. β) the function in Lemma 4.3. A similar computation as in *(iii)* gives that

$\int_{\mathbb{R}^2} \underline{u}_m \, \overline{\underline{v}_m} \, \mathrm{d}x = z_0 \, h + \mathcal{O}\left(h^2\right)$ where

$$z_0 = \sum_{\pm} \int_{\mathbb{T}_L} \alpha(s)\overline{\beta(s)} \mathrm{e}^{\mathrm{i}\theta_1(s) - \mathrm{i}\overline{\vartheta_1(s)}} \int_{\mathbb{R}_\pm} \mathrm{e}^{\mp 2\rho \, \widehat{\tau}_0(s) \eta_0(s)^{\mp 1}} \, \mathrm{d}\rho \, \mathrm{d}s$$

$$= \int_{\mathbb{T}_L} \alpha(s)\overline{\beta(s)} \, \mathrm{e}^{\mathrm{i}\theta_1(s) - \mathrm{i}\overline{\vartheta_1(s)}} \, \frac{\eta_0(s)^{-1} + \eta_0(s)}{2\widehat{\tau}_0(s)} \, \mathrm{d}s.$$

From the expression of θ_1 and ϑ_1 in Using Lemma B.2, we get $\mathrm{i}\theta_1(s) - \mathrm{i}\overline{\vartheta_1(s)} = -2f(s) - \int_0^s \frac{\alpha'(t)}{\alpha(t)} + \frac{\overline{\beta'(t)}}{\overline{\beta(t)}} \, \mathrm{d}t$ where f is a real function independent of α and β. A derivative computation shows that the functions

$$s \mapsto \alpha(s) \exp\left(-\int_0^s \frac{\alpha'(t)}{\alpha(t)} \, \mathrm{d}t\right) \equiv \alpha_0 \in \mathbb{C}^* \text{ and } s \mapsto \beta(s) \exp\left(-\int_0^s \frac{\beta'(t)}{\beta(t)} \, \mathrm{d}t\right) \equiv \beta_0 \in \mathbb{C}^*$$

are constant so $z_0 = \alpha_0 \overline{\beta_0} \int_{\mathbb{T}_L} \frac{\eta_0(s)^{-1} + \eta_0(s)}{2\widehat{\tau}_0(s)} \, \mathrm{e}^{-2f(s)} \, \mathrm{d}s \neq 0$. Denoting R (resp. S) the remainder in the construction of $\underline{u}_m$ (resp. $\underline{v}_m$), we have

$$\int_{\mathbb{R}^2} \underline{u}_m \, \underline{v}_m \, \mathrm{d}x = \int_{\mathbb{T}_L} F(h; s) \, \mathrm{e}^{\mathrm{i}\frac{4\pi m}{L}\theta_0(s)} \, \mathrm{d}s$$

where

$$F(h; s) = \mathrm{e}^{\mathrm{i}R_1^{\ominus}(h;s) + \mathrm{i}S_1^{\ominus}(h;s)}$$
$$\sum_{\pm} \int_{\mathbb{R}_\pm} \chi_u(h\rho)\chi_v(h\rho)R_0^{\pm}(h; s, \rho)S_0^{\pm}(h; s, \rho)h(1 + \rho\kappa(s)h) \, \mathrm{d}\rho.$$

Note that $F \in \mathscr{C}^\infty([0, \frac{L}{2\pi}] \times \mathbb{T}_L)$. Since $\theta_0' = \widehat{\tau}_0 > 0$, θ_0 is a smooth diffeomorphism form $\mathbb{T}_L$ to $\mathbb{T}_L$, we perform the change of variable $x = \theta_0(s)$

$$\int_{\mathbb{T}_L} F(h; s) \, \mathrm{e}^{\mathrm{i}\frac{4\pi m}{L}\theta_0(s)} \, \mathrm{d}s = \int_{\mathbb{T}_L} (\theta_0^{-1})'(x) \, F(h; \theta_0^{-1}(x)) \, \mathrm{e}^{\mathrm{i}\frac{4\pi}{L}mx} \, \mathrm{d}x.$$

From the fact that the function $(h; x) \mapsto (\theta_0^{-1})'(x) \, F(h; \theta_0^{-1}(x)) \in \mathscr{C}^\infty([0, \frac{2\pi}{L}] \times \mathbb{T}_L)$ and the Riemann-Lebesgue lemma, we get

$$\int_{\mathbb{T}_L} (\theta_0^{-1})'(x) \, F(h; \theta_0^{-1}(x)) \, \mathrm{e}^{\mathrm{i}\frac{4\pi}{L}mx} \, \mathrm{d}x = \mathcal{O}(m^{-\infty}).$$

□

We now add a correction to $\underline{u}_m$ in order to satisfy the transmission conditions. Consider $(\underline{\lambda}_m, \underline{u}_m)_{m \geq 1}$ in Eq. (4.16), satisfying Lemma 4.9. We define

$$\check{\underline{u}}_m(s, \xi) = \chi(\xi) \begin{cases} 0 & \text{if } \xi \leq 0 \\ \left[\underline{u}_m\right]_{\mathbb{T}_L \times \{0\}}(s) + \xi \left[a^{-1} \, \partial_\xi \underline{u}_m\right]_{\mathbb{T}_L \times \{0\}}(s) & \text{if } \xi > 0 \end{cases}.$$

Using Lemma 4.9, we have $\|\check{\underline{u}}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}(m^{-\infty})$ therefore $\underline{u}_m - \check{\underline{u}}_m \in \mathcal{D}(P)$ and $(P - \underline{\lambda}_m)(\underline{u}_m - \check{\underline{u}}_m) = \mathcal{O}(m^{-\infty})$. We then replace $\underline{u}_m$ by

$$\underline{u}_m = \frac{\underline{u}_m - \check{\underline{u}}_m}{\|\underline{u}_m - \check{\underline{u}}_m\|_{\mathrm{L}^2(\mathbb{R}^2)}} \tag{4.21}$$

which now makes $(\underline{\lambda}_m, \underline{u}_m)_{m \geq 1}$ a quasi-pair in the sense of Definition 2.2. To prove Theorem 2.3, we simply need to show that $(\underline{\lambda}_m)_{m \geq 1}$ are real and independent of the construction. To that aim we will check that $(\check{\lambda}_n)_{n \geq 1}$ are real and unique (see Remark 4.7).

Lemma 4.12. *Let $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$ and $(\underline{\mu}_m, \underline{v}_m)_{m\geq 1}$ two quasi-pairs in the sense of Definition 2.2 corresponding to the same integer m and having the same leading order phase $\theta_0 : s \mapsto \int_0^s \widehat{\tau}_0(t)\,\mathrm{d}t$. Then we have the following estimate $\underline{\lambda}_m - \overline{\underline{\mu}_m} = \mathcal{O}\left(m^{-\infty}\right)$.*

Proof. Let $\underline{R}_m$, $\underline{S}_m$ be the residuals $\underline{R}_m = P\underline{u}_m - \underline{\lambda}_m\,\underline{u}_m$ and $\underline{S}_m = P\underline{v}_m - \underline{\mu}_m\,\underline{v}_m$. By definition, the residuals satisfy $\|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}(m^{-\infty})$ and $\|\underline{S}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}(m^{-\infty})$. Using the symmetry of the operator P, we get

$$\left(\underline{\lambda}_m - \overline{\underline{\mu}_m}\right)\int_{\mathbb{R}^2} \underline{u}_m\,\overline{\underline{v}_m}\,\mathrm{d}x = \int_{\mathbb{R}^2} \underline{u}_m\,\overline{\underline{S}_m}\,\mathrm{d}x - \int_{\mathbb{R}^2} \underline{R}_m\,\overline{\underline{v}_m}\,\mathrm{d}x = \mathcal{O}\left(m^{-\infty}\right).$$

From Remark 4.10 one can show that there exists $z_0 \in \mathbb{C}^*$ such that $\int_{\mathbb{R}^2} \underline{u}_m\,\overline{\underline{v}_m}\,\mathrm{d}x = z_0 + \mathcal{O}(m^{-1})$. Then $\underline{\lambda}_m - \overline{\underline{\mu}_m} = \mathcal{O}(m^{-\infty})$ as $m \to +\infty$. □

Corollary 4.13. *The quasi-resonances $(\underline{\lambda}_m)_{m\geq 1}$ are real and are independent of the construction.*

Proof. By applying Lemma 4.12 to $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$ and $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$ we get $\Im\underline{\lambda}_m = \mathcal{O}(m^{-\infty})$ which implies that $\Im\breve{\lambda}_n = 0$ for all $n \in \mathbb{N}$. Then taking $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$ and $(\underline{\mu}_m, \underline{v}_m)_{m\geq 1}$ two quasi-pairs in the sense of Definition 2.2, from Remark 4.5, we can always assume that they have the same leading phase $\theta_0 : s \mapsto \int_0^s \widehat{\tau}_0(t)\,\mathrm{d}t$ (by taking $\overline{\underline{v}_m}$ instead of $\underline{v}_m$). Therefore, Lemma 4.12 and the fact that the quasi-resonances are real give us $\underline{\lambda}_m - \underline{\mu}_m = \mathcal{O}(m^{-\infty})$, which implies that $\breve{\lambda}_n = \breve{\mu}_n$. □

Results from Corollary 4.13, Lemma 4.9 and Eq. (4.21) imply Theorem 2.3. In the next section we use Theorem 2.3 and the black box scattering theory to prove Theorem 2.4, Corollary 2.5, Corollary 2.6, to establish the connection between the quasi-pairs and the scattering resonances, plus their effect on the scattering instabilities. We end this section with a few remarks.

Remark 4.14. With Corollary 4.13, given a quasi-pair $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$, we have a second quasi-orthogonal quasi-pair $(\underline{\lambda}_m, \overline{\underline{u}_m})_{m\geq 1}$ with the same quasi-resonance in the sense that, from *(v)* in Lemma 4.9, $\int_{\mathbb{R}^2} \underline{u}_m\,\overline{\overline{\underline{u}_m}}\,\mathrm{d}x = \mathcal{O}\left(m^{-\infty}\right)$. The quasi-resonances have an asymptotic multiplicity of 2, related to the chosen sign of the leading phase θ_0 (see Remark 4.5).

Remark 4.15. We can generalize the hypothesis of Theorem 2.3 to complex-valued function $a_{\mathsf{c}} \in \mathscr{C}^\infty(\overline{\Omega}, \mathbb{C}^*)$ as long as $a_{\mathsf{c}}|_\Gamma \neq -1$ and $\rho \mapsto \varphi_0^\pm(s,\rho)$ in Lemma 4.3 are exponentially decreasing for $\rho \to \pm\infty$. In other words we need

$$\Re\left(\widehat{\tau}_0(s)\,\eta_0(s)^{\pm 1}\right) > 0 \qquad \text{where } \tau_0(s) = \left(1 - \eta_0(s)^{-2}\right)^{-\frac{1}{2}} \text{ and } \widehat{\tau}_0 = \frac{\tau_0}{\langle \tau_0 \rangle}$$

and considering the principal branch of the square root. However, if a_{c} is complex non-real, the operator P is non-self-adjoint and Lemma 4.12, Corollary 4.13, Remark 4.14 are not true anymore.

4.4. **First expansion terms of $\underline{\lambda}_m$.** We provide here a few terms of the asymptotic expansions of $\underline{\lambda}_m$ to identify their key features. The coefficients $\breve{\lambda}_n$ are computed using formulas in the proof of Lemma 4.6 via SymPy [31], and symbolic codes are available in the Github repository [34].

General cavity with varying coefficient. We set the coefficients $\eta_0(s) = \eta(s,0)$ and $\eta_1(s) = \partial_\xi\eta(s,0)$, we obtain

$$\underline{\lambda}_m = \left(\frac{2\pi m}{L}\right)^2 \frac{\varsigma}{\langle\tau_0\rangle^2}\left[1 - \left\langle \frac{\eta_0^2 - 1}{\eta_0}\kappa + \frac{\eta_1}{{\eta_0}^2({\eta_0}^2 - 1)} \right\rangle \left(\frac{L}{2\pi m}\right) + \mathcal{O}\left(m^{-2}\right)\right]. \qquad (4.22)$$

Looking at the first terms one can see that:

- The sign comes from the leading term and depends on $a_{\mathsf{c}} < -1$ or $-1 < a_{\mathsf{c}} < 0$.
- The curvature κ appears only starting at the second term, it has a weak effect on the expansion.
- The terms blow up in the limit $\eta_0 \to 1$ (which correspond to $a_{\mathsf{c}} \to -1$). This is expected as for $a_{\mathsf{c}} \equiv -1$ since surface plasmon waves correspond to zero eigenvalues.

One can compute higher order terms such as $\breve{\lambda}_2$, however it becomes rather cumbersome and lengthy to present here (expressions can be found in [34]). We provide below a specific case where the expression $\breve{\lambda}_2$ is not too large.

Circular cavity of radius R with radially varying coefficient $\eta(r)$. Following previous results, we then set $\eta_0 = \eta(R)$, $\eta_1 = \partial_r \eta(R)$, $\eta_2 = \partial_r^2 \eta(R)$, and we obtain

$$\underset{\sim}{\lambda}_m = \frac{m^2}{R^2}\left(1-\eta_0^{-2}\right)\left[1 - \left(\frac{\eta_0^2-1}{\eta_0 R} + \frac{\eta_1}{\eta_0^2(\eta_0^2-1)}\right)\left(\frac{R}{m}\right) + \breve{\lambda}_2\left(\frac{R}{m}\right)^2 + \mathcal{O}\left(m^{-2}\right)\right] \quad (4.23)$$

where

$$\breve{\lambda}_2 = -\frac{(\eta_0^4+1)(\eta_0^4-\eta_0^2+1)}{2\eta_0^4R^2} + \frac{\eta_1(\eta_0^8+2\eta_0^6-3\eta_0^2+2)}{5\eta_0^5(\eta_0^4-1)R} - \frac{\eta_1^2(3\eta_0^4+4\eta_0^2-1)}{2\eta_0^6(\eta_0^4-1)} + \frac{\eta_2}{2\eta_0^3(\eta_0^2-1)}.$$

5. Black Box Scattering Theory for unbounded transmission problems with sign-changing coefficient

5.1. **Proof of Theorem 2.4.** In this section we prove Theorem 2.4, which is a consequence of the theorem of Tang and Zworski (see [42]) from the black box scattering framework. The proof is a direct consequence of the following elements:

- the operator $(P, \mathcal{D}(P))$ is a *black box Hamiltonian* in the sense of [20, Definition. 4.1] (see Lemma 5.2);
- one can estimate the number of eigenvalues of the reference operator $P^\sharp$ (a truncated version of the operator P) defined in Definition 5.3 (see Lemma 5.4). This allows to establish that the set of resonances, which is discrete, is not too large (one can count them).

Remark 5.1. From Remark 4.14, we have two quasi-orthogonal quasi-pairs and, as in [6, Theorem 7.D], we have two resonances close to the quasi-resonance. This will be illustrated in Section 6.

In what follows we prove Lemma 5.2 and Lemma 5.4. Let us denote $\mathbb{D} := B(0, R_0)$ the open disk of radius R_0 so that the cavity Ω is compactly embedded in $\mathbb{D}$. We denote $\mathbf{1}_{\mathbb{D}}$, $\mathbf{1}_{\mathbb{R}^2\setminus\overline{\mathbb{D}}}$ the restriction on $\mathbb{D}$, $\mathbb{R}^2 \setminus \overline{\mathbb{D}}$, respectively.

Lemma 5.2. *The operator $(P, \mathcal{D}(P))$ on $\mathrm{L}^2(\mathbb{R}^2)$ is a black box Hamiltonian in the sense of* [20, Definition. 4.1]*, meaning that the following is satisfied:*

(4.1.1): *we have the orthogonal decomposition* $\mathrm{L}^2(\mathbb{R}^2) = \mathrm{L}^2(\mathbb{D}) \oplus \mathrm{L}^2(\mathbb{R}^2 \setminus \overline{\mathbb{D}})$.

(4.1.4): *the operator $(P, \mathcal{D}(P))$ is self-adjoint and* $\mathbf{1}_{\mathbb{R}^2\setminus\overline{\mathbb{D}}}\mathcal{D}(P) \subset \mathrm{H}^2(\mathbb{R}^2 \setminus \overline{\mathbb{D}})$.

(4.1.5): *outside of $\mathbb{D}$ the operator is equal to the Laplacian.*

(4.1.6): *for all $v \in \mathrm{H}^2(\mathbb{R}^2)$ such that $v|_{B(0,R_0+\varepsilon)} \equiv 0$ for $\varepsilon > 0$ then $v \in \mathcal{D}(P)$.*

(4.1.12): *the operator* $\mathbf{1}_{\mathbb{D}}\,(P + \mathrm{i})^{-1} : \mathrm{L}^2(\mathbb{R}^2) \to \mathrm{L}^2(\mathbb{D})$ *is compact.*

Proof. The condition (4.1.1) is satisfied by definition. The condition (4.1.4) is a consequence of Lemma A.3 and Footnote 1. The condition (4.1.5) is satisfied by definition of $(P, \mathcal{D}(P))$: $\mathbf{1}_{\mathbb{R}^2\setminus\overline{\mathbb{D}}}(Pu) = -\Delta\left(\mathbf{1}_{\mathbb{R}^2\setminus\overline{\mathbb{D}}}(u)\right)$ for $u \in \mathcal{D}(P)$. The condition (4.1.6) is a consequence of Footnote 1. For the condition (4.1.12), we define $A : \mathrm{L}^2(\mathbb{R}^2) \to \mathrm{L}^2(\mathbb{D})$, $u \mapsto \iota\, \mathbf{1}_{\mathbb{D}}\,(P + \mathsf{i})^{-1}$, with the embedding $\iota : \mathrm{H}^1(\mathbb{D}) \to \mathrm{L}^2(\mathbb{D})$. The operator A is compact because $-\mathsf{i}$ is in the resolvent set (Lemma A.3), the projection $\mathbf{1}_{\mathbb{D}}$ goes from $\mathcal{D}(P)$ to $\mathrm{H}^1(\mathbb{D})$ (Footnote 1), and ι is compact [15, Thm. 9.16]. □

Now that the operator $(P, \mathcal{D}(P))$ is a black box Hamiltonian, the solutions of Eq. (2.3) are well-defined. Then we define the reference operator and estimate its eigenvalues. From Lemma 5.2 we deduce that Conditions (1), (2), (3) in [42] are satisfied. Lemma 5.4 establishes that the last condition, Condition (4) in [42], is satisfied.

Definition 5.3. From the operator $(P, \mathcal{D}(P))$ on $\mathrm{L}^2(\mathbb{R}^2)$, we define the reference operator $(P^\sharp, \mathcal{D}(P^\sharp))$ on $\mathrm{L}^2\left((\mathbb{R}/R_\sharp\mathbb{Z})^2\right)$ with $R_\sharp > R_0$ by $P^\sharp : u \mapsto -\operatorname{div}\left(a_\sharp^{-1}\nabla u\right)$ and

$$\mathcal{D}(P^\sharp) = \left\{u \in \mathrm{L}^2\left((\mathbb{R}/R_\sharp\mathbb{Z})^2\right) \;\middle|\; P^\sharp u \in \mathrm{L}^2\left((\mathbb{R}/R_\sharp\mathbb{Z})^2\right)\right\}$$

where $a_\sharp = a_{\mathsf{c}}\,\mathbf{1}_{\overline{\Omega}} + \mathbf{1}_{(\mathbb{R}/R_\sharp\mathbb{Z})^2\setminus\overline{\Omega}}$ is the “restriction” of a to $(\mathbb{R}/R_\sharp\mathbb{Z})^2$.

Lemma 5.4. *The reference operator $(P^\sharp, \mathcal{D}(P^\sharp))$ is self-adjoint, has discrete spectrum, and we have the following weak Weyl estimate*

$$\operatorname{Card}\left(\operatorname{Spec}(P^\sharp) \cap [-\mu, \mu]\right) = \mathcal{O}(\mu) \qquad \text{for } \mu \geq 1.$$

Proof. The proof that the reference operator is self-adjoint is the similar as in the proof of Lemma A.3 (see also [16, Theorem 4.2]). The spectrum is discrete because $(\mathbb{R}/R_\sharp\mathbb{Z})^2$ is a compact set. The weak Weyl estimation comes from [30, Section. 3], particularly from Corollary 8. The proofs are the same, one simply replaces $\mathrm{H}^1_0(\Omega)$ by the zero mean function in $\mathrm{H}^1\left((\mathbb{R}/R_\sharp\mathbb{Z})^2\right)$. □

Lemma 5.4 shows that Condition (4) in [42] is satisfied with $n^\sharp = 2$. Now that the resonance set is well-defined and characterized by quasi-pairs, we can prove Corollary 2.5. We will use the following result:

Lemma 5.5. *For $k \in \mathbb{C}\setminus\mathbb{R}_-$, we denote $\mathfrak{Res}(k) : \mathrm{L}^2_{\mathrm{comp}}(\mathbb{R}^2) \to \mathcal{D}_{\mathrm{loc}}(P)$ the meromorphic continuation of the resolvent. For $k > 0$ and $\chi \in \mathscr{C}^\infty_{\mathrm{comp}}(\mathbb{R}^2)$, we define $\mathfrak{Res}_\chi(k) : \mathrm{L}^2(\mathbb{R}^2) \to \mathcal{D}(P)$ the cut-off resolvent by $\mathfrak{Res}_\chi(k) = \chi\mathfrak{Res}(k)\chi$, as in* [32, Section. 3.2].

Proof. The meromorphic continuation of the resolvent is given by Theorem 4.4 in [20] and Lemma 5.2. □

5.2. **Proof of Corollary 2.5.** Let $\chi \in \mathscr{C}^\infty_{\mathrm{comp}}(\mathbb{R}^2)$ with $\chi \equiv 1$ on an open neighborhood of $\overline{\Omega}$. From the definition of the quasi-pair $(\underline{\lambda}_m, \underline{u}_m)_{m\geq 1}$, let $\underline{k}_m = \sqrt{\underline{\lambda}_m}$ and $\underline{v}_m = \chi\underline{u}_m$. The family $(\underline{k}_m^2, \underline{v}_m)_{m\geq 1}$ is still a quasi-pair, therefore, we have $P\underline{v}_m - \underline{k}_m^2\underline{v}_m = \underline{R}_m$ with the estimation $\|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}(m^{-\infty})$. This gives $\underline{u}_m = \mathfrak{Res}_\chi(\underline{k}_m)(\chi\underline{R}_m)$ so, for all $N \in \mathbb{N}$, there exists $C_N > 0$ such that

$$1 = \|\underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = \|\mathfrak{Res}_\chi(\underline{k}_m)(\chi\underline{R}_m)\| \leq \|\mathfrak{Res}_\chi(\underline{k}_m)\| C_N^{-1} m^{-N}$$

which gives the result.

5.3. **Proof of Corollary 2.6.** Now let $\underline{k}_m := \sqrt{\underline{\lambda}_m} \in \mathbb{C}^{\frac{1}{2}}$ for $m \geq 1$. Results from Section 4 give us $-\operatorname{div}(a^{-1}\nabla \underline{u}_m) - \underline{k}_m^2 \underline{u}_m = \underline{R}_m$ with the remainder estimate $\|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}(m^{-\infty})$. Lemma A.2 with $g = 0$ and $f = \underline{R}_m$, gives us

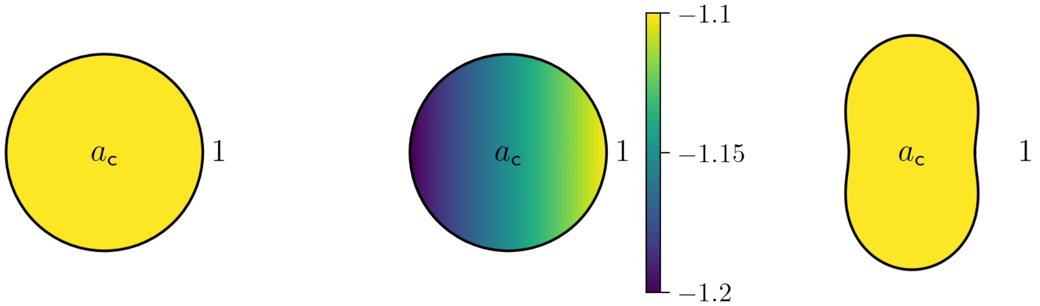
$$\|\underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} \leq C(\underline{k}_m)\ \|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2)}\,.$$

Since $\|\underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = 1$ by definition and for all $N \geq 1$, there exists $\widetilde{c}_N > 0$ such that $\|\underline{R}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} \leq \widetilde{c}_N m^{-N}$ then $\widetilde{c}_N^{-1}\, m^N \leq C(\underline{k}_m)$, for all $m \geq 1$.

6. Numerical illustration of metamaterial scattering resonances

Using Theorem 2.4 and Corollary 2.5 (proved in Section 5), we now have a way to identify and characterize scattering resonances ℓ, induced by surface plasmon waves. Those scattering resonances exist when $a_{\mathsf{c}}(\gamma) < -1$ for all $\gamma \in \Gamma$, and are located close to the real axis. Choosing $k = \Re(\ell)$ will lead to scattering instabilities for Eq. (2.2). In what follows we provide several numerical examples showing the norm of the resolvant operator exploding close to scattering resonances. First we use the Finite Element Method (FEM) to compute the scattering resonances ℓ of the cavity close to the real axis, then we compute the norm of the discretized cut-off resolvent operator for various k. We provide details below about the two steps. We consider three cases:

(A) Circular cavity of radius 1 with constant $a_{\mathsf{c}} \equiv -1.1$ as represented in Fig. 7a.
(B) Circular cavity of radius 1 with linearly varying permittivity $a_{\mathsf{c}}^{a_{\mathsf{m}},a_{\mathsf{M}}} \colon (x,y) \mapsto \frac{a_{\mathsf{m}}+a_{\mathsf{M}}}{2} + \frac{a_{\mathsf{M}}-a_{\mathsf{m}}}{2}x$, with $(a_{\mathsf{m}}, a_{\mathsf{M}}) = (-1.2, -1.1)$, as represented in Fig. 7b.
(C) Peanut cavity with constant $a_{\mathsf{c}} \equiv -1.1$ as represented in Fig. 7c. The peanut boundary is parameterized by $r(\theta) = 1 - \frac{3}{10}\cos(2\theta)$ with $\theta \in \mathbb{R}/2\pi\mathbb{Z}$.

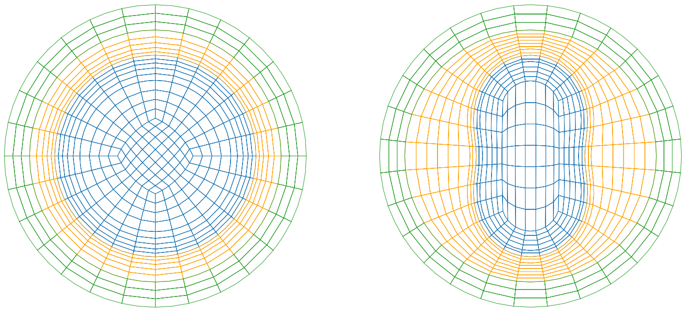


(A) Disk *(B) Disk, varying a_{c}* *(C) Peanut*

Figure 7. *Sketch representing the three considered configurations (A), (B), and (C), for the numerical illustration.*

Step 1: computing resonances. In order to solve Eq. (2.3), we truncate the computational domain with a circular *perfectly matched layer* (PML) as done in [33] (represented in green in Fig. 8), and we consider T-conforming meshes (ad hoc locally symmetric meshes along the interface Γ) to guarantee FEM optimal convergence and avoid spurious eigenvalues [17, 9]. In practice, we build such meshes using GMSH [22] and consider quadrangular elements of degree 3 embedded in a tubular neighborhood as defined in Eq. (4.1). We build a circular PML with radii $r_0 = 1.25$, $r_1 = r_0 + 0.25$ for the disk, and $r_0 = 1.25 \times 1.3$, $r_1 = r_0 + 0.25 \times 1.3$ for the peanut.

The FEM computations are done using finite elements of degree 8 using `XLife++` [43], leading to 33 713 degrees of freedom for all three cases. Table 1 contains computed scattering resonances values ℓ_{fem} for various numbers of curvilinear oscillations $m \in \{3, 6, 12\}$, for the three cases. As mentioned in Remarks 4.5, 4.14 and 5.1, for a given m, there are



Mesh for the disk *Mesh for the peanut*

Figure 8. *Structured mesh for the circular cavity (left) and the peanut shape cavity (right). The cavity is represented in blue, the exterior domain in orange, and the PML in green. The mesh is locally symmetric along the interface* Γ.

two resonances. We plot in Fig. 9 the two associated resonant modes for cases (B) and (C) associated to $m = 12$. One can observe that the size of angular oscillations changes when a_{c} varies (case (B)).

ℓ_{fem}	$m = 3$	$m = 6$	$m = 12$
(A)	$1.1472 - \mathrm{i}10^{-2}$	$2.072 - \mathrm{i}10^{-3}$	$3.89308 - \mathrm{i}10^{*}$
	$1.1472 - \mathrm{i}10^{-2}$	$2.072 - \mathrm{i}10^{-3}$	$3.89308 - \mathrm{i}10^{*}$
(B)	$0.966 - \mathrm{i}10^{-1.6}$	$2.0681 - \mathrm{i}10^{-2}$	$4.21203 - \mathrm{i}10^{-5}$
	$0.966 - \mathrm{i}10^{-1.6}$	$2.0681 - \mathrm{i}10^{-2}$	$4.21231 - \mathrm{i}10^{-5}$
(C)	$0.46 - \mathrm{i}10^{-0.86}$	$1.5455 - \mathrm{i}10^{-1.91}$	$3.2954955 - \mathrm{i}10^{-3.32}$
	$0.93 - \mathrm{i}10^{-1.49}$	$1.6912 - \mathrm{i}10^{-2.65}$	$3.2990404 - \mathrm{i}10^{-4.44}$

Table 1. *Approximate value of the scattering resonances* ℓ_{fem} *in the three cases and for* $m \in \{3, 6, 12\}$. *The number of digits displayed is evaluated using an estimated numerical error, and we have put a "*" when the value is below the estimated error.*

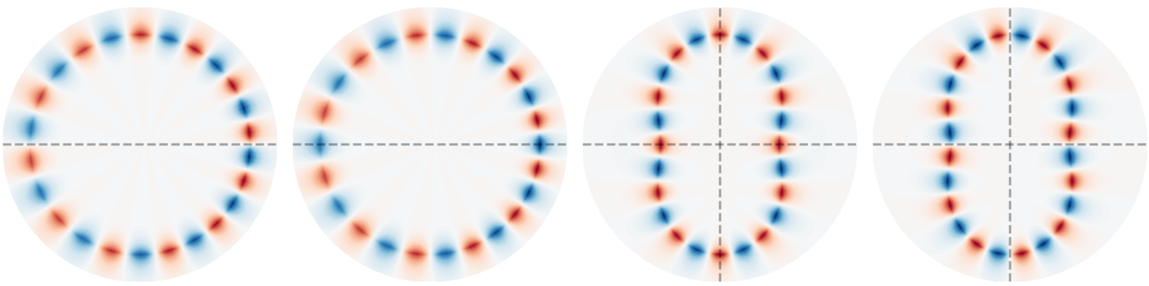
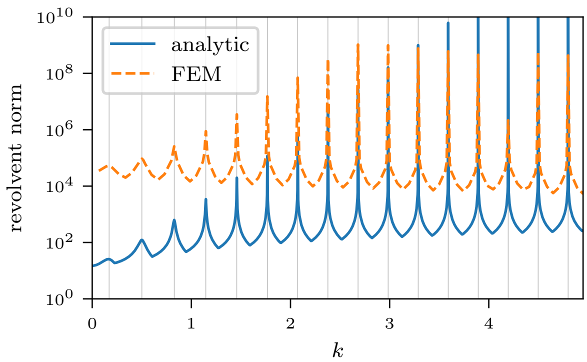


Figure 9. *Real part of the 2 resonant modes associated to* $m = 12$ *curvilinear oscillations, associated to the resonances in Table 1: for case (B) (left, middle left), for case (C) (middle right, right). The gray dashed lines represent the symmetry axes of the problem and hence the symmetries of the modes.*

Step 2: norm of the discretized cut-off resolvent operator. In Section 3 we computed the discrete norm of the reduced cut-off resolvent operator $|||\mathbb{A}_k^{-1}|||_2$, obtained using separation of variables. Here, we compute the discrete norm of a finite element version of the resolvent operator. We equivalently rewrite Eq. (2.2) on a bounded domain using a Dirichlet-to-Neumann map (DtN), leading to Eq. (A.3) presented in Appendix A. We use FEM with T-conforming meshes such as the ones in Fig. 8 but without the PML to approximate Eq. (A.3), and we denote $\mathbb{M}_k$ the finite element matrix of the associated operator. Then we compute the associated discrete norm $|||\mathbb{M}_k^{-1}|||_2$ of the finite element cut-off resolvent operator using the spectral norm by a power method on $(\mathbb{M}_k^{\intercal})^{-1}\mathbb{M}_k^{-1}$ on a uniform k-grid with geometric refinement around the real part of the scattering resonances.

The FEM computations are done using finite elements of degree 8 (leading to 28 337 degrees of freedom for all three cases), 65 Fourier modes for the DtN [36], and k-grids of 160 elements for case (A), 150 elements for cases (B), (C) respectively.

Figure 10 presents results for case (A), where we can compare $|||\mathbb{M}_k^{-1}|||_2$ (dashed orange line) with $|||\mathbb{A}_k^{-1}|||_2$ (blue line) from the analytic computations in Section 3. Note that the numerical schemes used in both cases are not the same, hence we do not expect the results to identically match. However, the sharp peaks coincide exactly, they occur at $k = \Re(\ell_{\mathsf{fem}})$ (ℓ_{fem} being the FEM scattering resonances computed in Step 1), and they exponentially grow as k increases (the y-axis is on a logarithmic scale). The gray vertical lines correspond to the real part of the scattering resonances ℓ_{fem}. For larger wavenumbers k, the FEM captures the scattering instabilities, but it fails to capture the peaks' intensity. This is due to the fact that the mesh is in this case not refined enough (despite high FEM order).

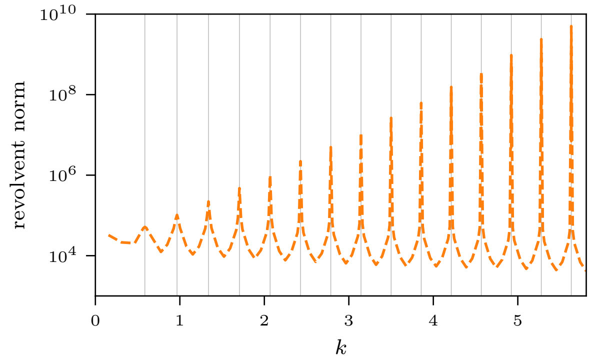


Case (A)

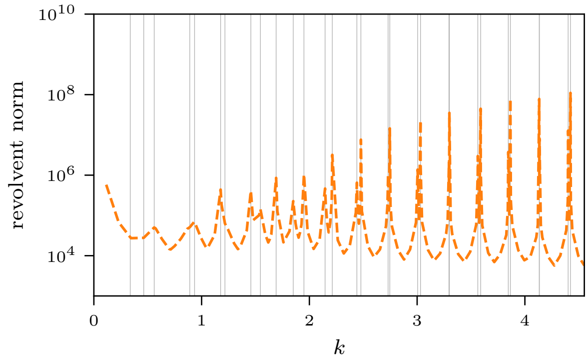
Figure 10. *Semi-log plot of the function $k \mapsto \|\mathbb{M}_k^{-1}\|_2$ for the disk cavity with $a_{\mathsf{c}} = -1.1$. The blue line correspond to the same analytic computation as in Section 3. The dotted orange lines correspond to FEM computations. The vertical grid lines are aligned on the real part of the scattering resonances.*

Figure 11 presents results for cases (B), (C), where we do not have an analytic computation to compare to. As before, we observe that the norm of the cut-off resolvent operator peaks for $k = \Re(\ell_{\mathsf{fem}})$ (indicated by the gray vertical lines in the figures), and the peaks grow exponentially with respect to k. As mentioned before, we have two resonant modes corresponding to the same number of curvilinear oscillations m, but they might have slightly different true resonances. For case (C), we clearly observe this phenomenon (double peaks). Note that for small m (i.e. small real part of the scattering resonances), the norm of the resolvent does not explode. This is due to scattering resonances having a more significant imaginary part.

Numerical results above illustrate the effect of scattering resonances induced by surface plasmon waves, for various metamaterial cavities (in shape and in coefficient).



Case (B)



Case (C)

Figure 11. *Semi-log plot of the function* $k \mapsto \left\|\mathbb{M}_k^{-1}\right\|_2$ *in logarithmic scale for the two cases* (B) *and* (C)*. The vertical grid lines are aligned on the real part of the scattering resonances.*

7. Conclusion

Similar to classical optical cavities, the scattering by negative metamaterial cavities can be significantly affected by localized waves at the boundary of the cavity. In this paper we have shown with the black box scattering framework that there exist metamaterial scattering resonances close to the real axis, causing the norm of resolvent operator to explode. Using asymptotic expansions, we have characterized those resonances and associated resonant modes, to arbitrary order, and for various cavity properties (arbitrary smooth shape, varying negative permittivity, etc.). It turns out, scattering resonances are associated to localized waves corresponding to surface plasmons waves. This study has been carried out without reducing to the quasi-static case, and the considered spectral parameter is the wavenumber in contrast to [23, 41, 1, 2]. Our asymptotic analysis revealed that, given some incident source associated to $k > 0$, surface plasmon waves can only be excited when $a_{\mathsf{c}} < -1$ (in the case $-1 < a_{\mathsf{c}} < 0$ the scattering resonances are purely imaginary). We have established that the existence of quasi-pairs implies the existence of scattering resonances close to the positive real axis which also implies the explosion of the stability constant when $a_{\mathsf{c}} < -1$. FEM computations confirm that the norm of the numerical resolvent operator exhibits high intensity narrow peaks associated to the scattering resonances close to the positive real axis.

Our approach provides an asymptotic characterization of emerging surface plasmon waves for general metamaterial cavities, to arbitrary order. One could consider extracting those asymptotic plasmonic behaviors from the problem to relax FEM (no peaks), as done in the singular complement method [19]. One could also, using the same expansion methods, find asymptotic characterization in the context of dispersive material cavities (in particular the case where $a_{\mathsf{c}} := \varepsilon_{\mathsf{c}}$ is the permittivity and depends on the wavenumber k, such as Drude's or Lorentz' model). In that case, our analysis confirms that surface plasmons waves can only be excited for frequencies lower than the surface plasmon frequency [29], however, since the domain of the operator depends on the spectral parameter, the link between quasi-pairs and scattering resonances is not clear. Extensions to polygonal metamaterial cavities and dispersive metamaterials will be considered. In the quasi-static case, the spectral analysis for that case reveals hypersingular plasmonic behaviors and has been well investigated [24, 13]. The proposed asymptotic expansions approach is valid for arbitrary optical parameter a_{c} (and complex-valued ones to some extent), one could also consider arbitrary double negative optical parameters b_{c} and work with the double-negative PDE $-\operatorname{div}(a^{-1}\nabla u) - b\,k^2\,u = 0$ (e.g. [11, 21, 3]). Then, to deduce from the quasi-pairs existence the presence of scattering resonances becomes difficult because the operator is no longer self-adjoint. All the derivation has been provided for two-dimensional problems, one could consider three-dimensional cavities.

Acknowledgments

The authors would like to thank C. Tsogka, A. D. Kim, and M. Dauge for theirs helpful feedback.

Funding

This research was supported by the National Science Fundation Grant: DMS-2009366 and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) — Project-ID 258734477 — SFB 1173.

References

[1] H. Ammari, Y. T. Chow, and H. Liu. Quantum ergodicity and localization of plasmon resonances, 2020. arXiv:2003.03696. URL: http://arxiv.org/abs/2003.03696.

[2] H. Ammari, A. Dabrowski, B. Fitzpatrick, and P. Millien. Perturbation of the scattering resonances of an open cavity by small particles. Part I: the transverse magnetic polarization case. *Zeitschrift für angewandte Mathematik und Physik*, 71(4):102, 2020. doi:10.1007/s00033-020-01324-6.

[3] H. Ammari, B. Fitzpatrick, H. Lee, S. Yu, and H. Zhang. Double-negative acoustic metamaterials. *Quarterly of Applied Mathematics*, 77(4):767–791, 2019. doi:10.1090/qam/1543.

[4] H. Ammari, P. Millien, M. Ruiz, and H. Zhang. Mathematical Analysis of Plasmonic Nanoparticles: The Scalar Case. *Archive for Rational Mechanics and Analysis*, 224:597–658, 2017. doi:10.1007/s00205-017-1084-5.

[5] V. M. Babic and V. S. Buldyrev. *Short-Wavelength Diffraction Theory: Asymptotic Methods*. Springer Series on Wave Phenomena. Springer-Verlag, Berlin Heidelberg, 1972.

[6] S. Balac, M. Dauge, and Z. Moitier. Asymptotics for 2D whispering gallery modes in optical micro-disks with radially varying index. *IMA Journal of Applied Mathematics*, 2021. doi:10.1093/imamat/hxab033.

[7] C. Bernardi, M. Dauge, and Y. Maday. *Spectral methods for axisymmetric domains*, volume 3 of *Series in Applied Mathematics (Paris)*. Gauthier-Villars, Éditions Scientifiques et Médicales Elsevier, Paris; North-Holland, Amsterdam, 1999. Numerical algorithms and tests due to Mejdi Azaïez.

[8] A.-S. Bonnet-Ben Dhia, C. Carvalho, L. Chesnel, and P. Ciarlet, Jr. On the use of perfectly matched layers at corners for scattering problems with sign-changing coefficients. *Journal of Computational Physics*, 322:224–247, 2016. doi:10.1016/j.jcp.2016.06.037.

[9] A.-S. Bonnet-Ben Dhia, C. Carvalho, and P. Ciarlet. Mesh requirements for the finite element approximation of problems with sign-changing coefficients. *Numerische Mathematik*, 138(4):801–838, 2018. doi:10.1007/s00211-017-0923-5.

[10] A.-S. Bonnet-Ben Dhia, L. Chesnel, and P. Ciarlet. T-coercivity for scalar interface problems between dielectrics and metamaterials. *ESAIM: Mathematical Modelling and Numerical Analysis*, 46(6):1363–1387, 2012. doi:10.1051/m2an/2012006.

[11] A.-S. Bonnet-Ben Dhia, L. Chesnel, and P. Ciarlet Jr. T-Coercivity for the Maxwell Problem with Sign-Changing Coefficients. *Communications in Partial Differential Equations*, 39(6):1007–1031, 2014. doi:10.1080/03605302.2014.892128.

[12] A.-S. Bonnet-Ben Dhia, L. Chesnel, and X. Claeys. Radiation condition for a non-smooth interface between a dielectric and a metamaterial. *Mathematical Models and Methods in Applied Sciences*, 23(09):1629–1662, 2013. doi:10.1142/s0218202513500188.

[13] A.-S. Bonnet-Ben Dhia, C. Hazard, and F. Monteghetti. Complex-scaling method for the complex plasmonic resonances of planar subwavelength particles with corners. *Journal of Computational Physics*, 440:110433, 2021. doi:10.1016/j.jcp.2021.110433.

[14] E. Bonnetier, C. Dapogny, F. Triki, and H. Zhang. The plasmonic resonances of a bowtie antenna. *Analysis in Theory and Applications*, 35(1):85–116, 2019. doi:10.4208/ata.OA-0011.

[15] H. Brezis. *Functional analysis, Sobolev spaces and partial differential equations*. Universitext. Springer, New York, 2011. doi:10.1007/978-0-387-70914-7.

[16] C. Carvalho. *Étude mathématique et numérique de structures plasmoniques avec coins*. Theses, ENSTA ParisTech, 2015. URL: https://pastel.archives-ouvertes.fr/tel-01240904.

[17] C. Carvalho, L. Chesnel, and P. Ciarlet Jr. Eigenvalue problems with sign-changing coefficients. *Comptes Rendus Mathematique*, 355(6):671–675, 2017. doi:10.1016/j.crma.2017.05.002.

[18] J. Cho, I. Kim, S. Rim, G.-S. Yim, and C.-M. Kim. Outer resonances and effective potential analogy in two-dimensional dielectric cavities. *Physics Letters A*, 374(17):1893–1899, 2010. doi:10.1016/j.physleta.2010.02.055.

[19] P. Ciarlet and J. He. The singular complement method for 2d scalar problems. *Comptes Rendus Mathematique*, 336(4):353–358, 2003. doi:10.1016/S1631-073X(03)00030-X.

[20] S. Dyatlov and M. Zworski. *Mathematical theory of scattering resonances*, volume 200 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2019. doi:10.1090/gsm/200.

[21] B. Fitzpatrick. *Mathematical Analysis of Minnaert Resonances for Acoustic Metamaterials*. PhD thesis, ETH Zurich, 2018. doi:10.3929/ethz-b-000287325.

[22] C. Geuzaine and J.-F. Remacle. Gmsh: A 3-d finite element mesh generator with built-in pre- and post-processing facilities. *International Journal for Numerical Methods in Engineering*, 79(11):1309–1331, 2009. doi:10.1002/nme.2579.

[23] D. Grieser. The plasmonic eigenvalue problem. *Reviews in Mathematical Physics*, 26(03):1450005, 2014. doi:10.1142/s0129055x14500056.

[24] C. Hazard and S. Paolantoni. Spectral analysis of polygonal cavities containing a negative-index material. *Annales Henri Lebesgue*, 3:1161–1193, 2020. doi:10.5802/ahl.58.

[25] J. Helsing and A. Karlsson. On a helmholtz transmission problem in planar domains with corners. *Journal of Computational Physics*, 371:315–332, 2018. doi:10.1016/j.jcp.2018.05.044.

[26] R. Hiptmair, A. Moiola, and E. A. Spence. Spurious quasi-resonances in boundary integral equations for the helmholtz transmission problem, 2021. arXiv:2109.08530.

[27] L. Hörmander. *The Analysis of Linear Partial Differential Operators I*, volume 256 of *Classics in Mathematics*. Springer Berlin Heidelberg, second edition, 2003. doi:10.1007/978-3-642-61497-2.

[28] P. Kravanja and M. Van Barel. *Computing the Zeros of Analytic Functions*. Springer Berlin Heidelberg, 2000. doi:10.1007/bfb0103928.

[29] S. A. Maier. *Plasmonics: Fundamentals and Applications*. Springer, New York, NY, 2007. doi:10.1007/0-387-37825-1.

[30] R. Mandel, Z. Moitier, and B. Verfürth. Nonlinear helmholtz equations with sign-changing diffusion coefficient, 2021. *to appear in Comptes Rendus - Mathématique*. arXiv:2107.14516.

[31] A. Meurer, C. P. Smith, M. Paprocki, O. Čertík, S. B. Kirpichev, M. Rocklin, A. Kumar, S. Ivanov, J. K. Moore, S. Singh, T. Rathnayake, S. Vig, B. E. Granger, R. P. Muller, F. Bonazzi, H. Gupta, S. Vats, F. Johansson, F. Pedregosa, M. J. Curry, A. R. Terrel, v. Roučka, A. Saboo, I. Fernando, S. Kulal, R. Cimrman, and A. Scopatz. Sympy: symbolic computing in python. *PeerJ Computer Science*, 3:e103, 2017. doi:10.7717/peerj-cs.103.

[32] A. Moiola and E. A. Spence. Acoustic transmission problems: wavenumber-explicit bounds and resonance-free regions. *Mathematical Models and Methods in Applied Sciences*, 29(2):317–354, 2019. doi:10.1142/S0218202519500106.

[33] Z. Moitier. *Étude mathématique et numérique des résonances dans une micro-cavité optique*. PhD thesis, Université de Rennes 1, 2019. Thèse de doctorat dirigée par Dauge, Monique et Balac, Stéphane Mathématiques et leurs interactions Rennes 1 2019. URL: http://www.theses.fr/en/2019REN1S053.

[34] Z. Moitier and C. Carvalho. Asymptotic_metacavity. https://github.com/zmoitier/Asymptotic_metacavity, 2021. https://doi.org/10.5281/zenodo.4716362.

[35] P. Moon and D. E. Spencer. *Field Theory Handbook: Including Coordinate Systems, Differential Equations and Their Solutions*. Springer-Verlag, Berlin Heidelberg, 2 edition, 1988.

[36] A. A. Oberai, M. Malhotra, and P. M. Pinsky. On the implementation of the Dirichlet-to-Neumann radiation condition for iterative solution of the Helmholtz equation. *Applied Numerical Mathematics*, 27(4):443–464, 1998. doi:10.1016/S0168-9274(98)00024-5.

[37] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, editors. *NIST handbook of mathematical functions*. U.S. Department of Commerce, National Institute of Standards and Technology, Washington, DC; Cambridge University Press, Cambridge, 2010. URL: https://dlmf.nist.gov/.

[38] G. C. Righini, Y. Dumeige, P. Féron, M. Ferrari, G. Nunzi Conti, D. Ristic, and S. Soria. Whispering gallery mode microresonators: Fundamentals and applications. *La Rivista del Nuovo Cimento*, 34(7):435–488, 2011. doi:10.1393/ncr/i2011-10067-2.

[39] P. Robert. cxroots: A Python module to find all the roots of a complex analytic function within a given contour, 2018–. URL: https://github.com/rparini/cxroots.
[40] T. Sannomiya, C. Hafner, and J. Voros. In situ sensing of single binding events by localized surface plasmon resonance. *Nano Letters*, 8(10):3450–3455, 2008. doi:10.1021/nl802317d.
[41] O. Schnitzer. Geometric quantization of localized surface plasmons. *IMA Journal of Applied Mathematics*, 84(4):813–832, 2019. doi:10.1093/imamat/hxz016.
[42] S.-H. Tang and M. Zworski. From quasimodes to resonances. *Mathematical Research Letters*, 5(3):261–272, 1998. doi:10.4310/MRL.1998.v5.n3.a1.
[43] XLiFE++. Librairie FEM-BEM C++, dévellopée conjointement par les laboratoires IRMAR et POems. https://uma.ensta-paristech.fr/soft/XLiFE++/, 2010–.

Appendix A. Properties of the operator P

We recall the operator $P\colon u \mapsto -\operatorname{div}(a^{-1}\nabla u)$. Given $\omega \subseteq \mathbb{R}^2$, we define the bilinear form

$$b_\omega(u,v) = \int_\omega a^{-1}\nabla u \cdot \nabla v \,\mathrm{d}x, \quad u,v \in \mathrm{H}^1(\omega). \tag{A.1}$$

Then $b := b_{\mathbb{R}^2}$ is the associated bilinear form of $(P, \mathcal{D}(P))$, one can write $b(u,v) = (Pu,v)_{\mathrm{L}^2}$ for $u \in \mathcal{D}(P)$, $v \in \mathrm{H}^1(\mathbb{R}^2)$, and is the associated bilinear form of Eq. (2.2) for $\mathtt{P}\colon \mathrm{H}^1(\mathbb{R}^2) \to \mathrm{H}^{-1}(\mathbb{R}^2)$ ($b(u,v) = \langle \mathtt{P}u, v\rangle$ for $u,v \in \mathrm{H}^1(\mathbb{R}^2)$, where $\langle\cdot,\cdot\rangle$ is the duality bracket $\mathrm{H}^{-1}(\mathbb{R}^2) \times \mathrm{H}^1(\mathbb{R}^2)$).

Lemma A.1. *If $a_{\mathsf{c}}(\gamma) \neq -1$, for all $\gamma \in \Gamma$, the bilinear form b_ω defined in Eq. (A.1) is weakly $\mathtt{T}$-coercive. More precisely, there exists an isomorphism $\mathtt{T} \in \mathcal{L}(\mathrm{H}^1(\omega))$, a compact operator $\mathtt{C} \in \mathcal{L}(\mathrm{L}^2(\omega))$, $\alpha > 0$, and $\beta \in \mathbb{R}$ such that b_ω satisfies a Gärding's inequality of the form:*

$$b_\omega(u, \mathtt{T}u) \geq \alpha \left\|u\right\|^2_{\mathrm{H}^1(\omega)} - \beta \left\|\mathtt{C}u\right\|^2_{\mathrm{L}^2(\omega)}, \quad \forall u \in \mathrm{H}^1(\omega).$$

Proof. When $a_{\mathsf{c}} < 0$ is constant, one can use $\mathtt{T}$ provided in [9] and the proof follows the one of [9, Lemma 2]. When $a_{\mathsf{c}} \in \mathscr{C}^\infty(\Omega)$ non-constant, since $\partial\Omega$ is a smooth interface, it can always be seen as locally straight, then Theorems 3.10 and 4.3 in [10] apply and provide the needed results. □

Lemma A.2. *If $a_{\mathsf{c}}(\gamma) \neq -1$, for all $\gamma \in \Gamma$, the operator $\mathtt{P}$ is Fredholm of index 0 and Eq. (2.2) is well-posed. Moreover, there exists a stability constant $C(k) > 0$ such that*

$$\left\|u\right\|_{\mathrm{L}^2(\mathbb{R}^2)} \leq C(k) \left(\left\|f\right\|_{\mathrm{L}^2(\mathbb{R}^2)} + \left\|g\right\|_{\mathrm{L}^2(\Gamma)} \right). \tag{A.2}$$

Proof. Let $\mathbb{D}(0,\rho)$ be a disk a radius ρ such that Ω is compactly embedded in $\mathbb{D}(0,\rho)$, and $f \in \mathrm{L}^2(\mathbb{D}(0,\rho))$. Following [8], we use a Dirichlet-to-Neumann map, denoted $\mathcal{S}$, to rewrite Eq. (2.2) in $\mathbb{D}(0,\rho)$: Find $u \in \mathrm{H}^1(\mathbb{D}(0,\rho))$ such that

$$\begin{cases} -\operatorname{div}\left(a^{-1}\nabla u\right) - k^2 u = f & \text{in } \mathbb{D}(0,\rho) \\ [u]_\Gamma = 0 \quad \text{and} \quad \left[a^{-1}\partial_n u\right]_\Gamma = g & \text{across } \Gamma \\ \partial_r u = \mathcal{S}u & \text{on } \partial\mathbb{D}(0,\rho) \end{cases} \tag{A.3}$$

Lemma 1 in [8] shows that problems Eq. (A.3)-Eq. (2.2) admits at most one solution. Following [8, Section 2], using the properties of $\mathcal{S}$ and the fact that $\mathtt{K}\colon u \mapsto -k^2 u$ is compact, one simply needs to establish that the operator $\mathtt{P}\colon u \mapsto -\operatorname{div}(a^{-1}\nabla u)$ is Fredholm to conclude. From [16, Proposition 2.6], it is equivalent to show that $b|_{\mathbb{D}(0,\rho)}$ in Eq. (A.1) is weakly $\mathtt{T}$-coercive, which is established by Lemma A.1. Well-posedness of Eq. (A.3) in Hadamard's sense gives u that there exists $\widetilde{C}(k) > 0$ such that

$$\left\|u\right\|_{\mathrm{H}^1(\mathbb{D}(0,\rho))} \leq \widetilde{C}(k) \left(\left\|g\right\|_{L^2(\Gamma)} + \left\|f\right\|_{\mathrm{L}^2(\mathbb{D}(0,\rho))} \right).$$

For Eq. (2.2), using Poincaré's inequality this leads to

$$\|u\|_{\mathrm{L}^2(\mathbb{R}^2)} \leq C(k)\left(\|g\|_{\mathrm{L}^2(\Gamma)} + \|f\|_{\mathrm{L}^2(\mathbb{R}^2)}\right). \tag{A.4}$$

□

Lemma A.3. *If $a_{\mathsf{c}}(\gamma) \neq -1$, for all $\gamma \in \Gamma$, then $(P, \mathcal{D}(P))$ is self-adjoint, and its spectrum is such that* $\operatorname{Spec}_{\mathrm{ess}}(P) = \mathbb{R}_+$ *and* $\operatorname{Spec}_{\mathrm{dis}}(P) \subset \mathbb{R}_-^*$.

Proof. The proof is given by applying Theorem 4.2, Propositions 4.5 and 4.6 in [16, Chapter 4]. Consider $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and the problem: Find $u \in \mathrm{H}^1(\mathbb{R}^2)$ such that $b(u,v) - \lambda(u,v)_{\mathrm{L}^2} = (f,v)_{\mathrm{L}^2}$, $\forall v \in \mathrm{H}^1(\mathbb{R}^2)$, with $f \in \mathrm{L}^2(\mathbb{R}^2)$. Using Lemma A.1, b is weakly $\mathtt{T}$-coercive and the above problem is well-posed (Lemma A.2). This shows that P is self-adjoint. Given $\lambda \in \operatorname{Spec}_{\mathrm{ess}}(P)$, consider $(u_n)_n \in \mathcal{D}(P)$ such $\|u_n\|_{\mathrm{L}^2(\mathbb{R}^2)} = 1$, $u_n \rightharpoonup 0$ weakly in L^2 and such that $\|Pu_n - \lambda u_n\|_{\mathrm{L}^2} \to 0$. Using Lemma A.1, we have

$$(Pu_n, \mathtt{T}u_n)_{\mathrm{L}^2(\mathbb{R}^2)} \geq \alpha \|u_n\|^2_{\mathrm{H}^1(\mathbb{R}^2)} - \beta \|\mathtt{C}u_n\|^2_{\mathrm{H}^1(\mathbb{R}^2)} \geq -\beta \|\mathtt{C}u_n\|^2_{\mathrm{L}^2(\mathbb{R}^2)}$$

and we note that

$$(Pu_n, \mathtt{T}u_n)_{\mathrm{L}^2(\mathbb{R}^2)} = \lambda(u_n, \mathtt{T}u_n)_{\mathrm{L}^2} = \lambda + \lambda(u_n, (\mathtt{T} - \mathrm{I})u_n)_{\mathrm{L}^2(\mathbb{R}^2)}.$$

Since $u_n \rightharpoonup 0$ weakly in L^2, one can show that $\|\mathtt{C}u_n\|^2_{\mathrm{L}^2(\mathbb{R}^2)} \to 0$, $(u_n, (\mathtt{T}-\mathrm{I})u_n)_{\mathrm{L}^2(\mathbb{R}^2)} \to 0$ strongly, which leads to $\lambda \geq 0$. On the other hand, for $\lambda \geq 0$, one can build a Weyl sequence $(u_n)_n \in \mathcal{D}(P)$ such $\|u_n\|_{\mathrm{L}^2(\mathbb{R}^2)} = 1$, $u_n \rightharpoonup 0$ weakly in L^2 and such that $\|Pu_n - \lambda u_n\|_{\mathrm{L}^2} \to 0$. Rellich lemma allows us to show that there are no eigenvalues in $\operatorname{Spec}_{\mathrm{ess}}(P)$. Finally, P doesn't admit a lower bound (details can be found in [16, Section 4.2.2]): one can consider a sequence $(u_n)_n \in \mathcal{D}(P)$ with support strictly included in Ω such that the numercial range $(Pu_n, u_n)_{\mathrm{L}^2} \to -\infty$ (recall that $a_{\mathsf{c}} < 0$), which shows that $\operatorname{Spec}_{\mathrm{dis}}(P) \subset \mathbb{R}_-^*$. □

Appendix B. Proofs and additional results for the asymptotic expansions

B.1. Proof of Lemma 4.3.

Proof. We solve Eq. (4.13) as ordinary differential equations with $s \in \mathbb{T}_L$ as a parameter. The conditions $\varphi_0^{\pm}(s,\cdot) \in \mathscr{S}(\mathbb{R}_{\pm})$ give the following restrictions $\theta_0'(s)^2 + \eta_0(s)^2\check{\lambda}_0 \in \mathbb{C}\setminus\mathbb{R}_-$ and $\theta_0'(s)^2 - \check{\lambda}_0 \in \mathbb{C} \setminus \mathbb{R}_-$. If one of the above restrictions is false, then there are no solutions $\varphi^{\pm}(s,\cdot)$ in $\mathscr{S}(\mathbb{R}_{\pm})$. Under those restrictions, there exists $\alpha(s), \beta(s) \in \mathbb{R}$ such that $\alpha(s)\beta(s) \neq 0$,

$$\varphi_0^-(s,\rho) = \alpha(s)e^{\rho\sqrt{\theta_0'(s)^2 + \eta_0(s)^2\check{\lambda}_0}}, \quad \text{and} \quad \varphi_0^+(s,\rho) = \beta(s)e^{-\rho\sqrt{\theta_0'(s)^2 - \check{\lambda}_0}},$$

where the square roots are chosen to be in $\mathbb{C}^{\frac{1}{2}}$. The first transmission condition $\varphi_0^-(s,0) = \varphi_0^+(s,0)$ implies that $\alpha(s) = \beta(s)$. Then the second transmission condition

$$-\eta_0(s)^{-2}\,\partial_\rho\varphi_0^-(s,0) = \partial_\rho\varphi_0^+(s,0)$$

give us

$$-\eta_0(s)^{-2}\sqrt{\theta_0'(s)^2 + \eta_0(s)^2\check{\lambda}_0} = -\sqrt{\theta_0'(s)^2 - \check{\lambda}_0},$$

leading to the eikonal equation

$$\theta_0'(s)^2 = \frac{\check{\lambda}_0}{1 - \eta_0(s)^{-2}} = \varsigma\check{\lambda}_0\,\left|1 - \eta_0(s)^{-2}\right|^{-1}.$$

While this equation does not have a unique solution, one simply selects one (see Remark 4.5). Here we choose

$$\theta_0(s) = \sqrt{\varsigma\check{\lambda}_0}\int_0^s \left|1-\eta_0(t)^{-2}\right|^{-\frac{1}{2}}\,\mathrm{d}t$$

and from the condition $\exp\left(\frac{\mathrm{i}}{h}\theta_0\right) \in \mathscr{C}^\infty(\mathbb{T}_L)$, we deduce that $\exp\left(\frac{\mathrm{i}}{h}\theta_0(L)\right) = \exp\left(\frac{\mathrm{i}}{h}\theta_0(0)\right)$ which implies that there exists $m \in \mathbb{N}$ such that

$$2\pi m = \frac{\theta_0(L)-\theta_0(0)}{h} = \frac{\sqrt{\varsigma\check{\lambda}_0}}{h}\int_0^L \left|1-\eta_0(t)^{-2}\right|^{-\frac{1}{2}}\,\mathrm{d}t.$$

By choosing $h = \frac{L}{2\pi m}$ for $m \in \mathbb{N}^*$, we get $1 = \sqrt{\varsigma\check{\lambda}_0}\left\langle \left|1-\eta_0^{-2}\right|^{-\frac{1}{2}}\right\rangle = \sqrt{\varsigma\check{\lambda}_0}\,\langle\tau_0\rangle$ which gives $\check{\lambda}_0 = \varsigma\,\langle\tau_0\rangle^{-2}$. Then with the relation $\tau_0^2 = \varsigma(1-\eta_0^{-2})^{-1}$ we obtain that

$$\sqrt{\theta_0'(s)^2 + \eta_0(s)^2\check{\lambda}_0} = \widehat{\tau}_0(s)\,\eta_0(s) > 0 \quad \text{and} \quad \sqrt{\theta_0'(s)^2 - \check{\lambda}_0} = \widehat{\tau}_0(s)\,\eta_0(s)^{-1} > 0,$$

which concludes the proof. □

B.2. Proof of Lemma 4.6.

Proof. For $(s,\rho) \in \mathbb{T}_L \times \mathbb{R}_\pm$, we define $\mathsf{e}^\pm(s,\rho) = \exp\left(-|\rho|\,\widehat{\tau}_0(s)\,\eta_0(s)^{\mp 1}\right)$. We proceed by induction on n. For $n=0$, Lemma 4.3 gives $(\varphi_0^\pm, \theta_0, \check{\lambda}_0)$ the solution of $(\mathcal{P}_0)$ defined in Eq. (4.13). Let $n \geq 1$, from the definition of $S_{n-1}^\pm$ in Eq. (4.15), there exists $Q_{n-1}^\pm \in \mathscr{C}^\infty(\mathbb{T}_L, \mathbb{P})$ such that $S_{n-1}^\pm = Q_{n-1}^\pm\,\mathsf{e}^\pm$. Using Lemma A.1 in [6], we can solve the two ODEs in Eq. (4.14) with the source terms $S_{n-1}^\pm$. We find that there exists $\widetilde{P}_n^\pm \in \mathscr{C}^\infty(\mathbb{T}_L, \mathbb{P})$ such that $\widetilde{\varphi}_n^\pm = \rho\widetilde{P}_n^\pm\,\mathsf{e}^\pm$, $\partial_\rho^2\widetilde{\varphi}_n^- - \widehat{\tau}_0^2\,\eta_0^2\,\widetilde{\varphi}_n^- = \eta_0^2\,S_{n-1}^-$, and $\partial_\rho^2\widetilde{\varphi}_n^+ - \widehat{\tau}_0^2\,\eta_0^{-2}\,\widetilde{\varphi}_n^+ = -S_{n-1}^+$. Then, solving the two ODEs in Eq. (4.14) with the source terms $(2\widehat{\tau}_0\theta_0' + \eta_0^2\check{\lambda}_n)\varphi_0^-$ and $(2\widehat{\tau}_0\theta_0' - \check{\lambda}_n)\varphi_0^-$, for $(s,\rho) \in \mathbb{T}_L \times \mathbb{R}_\pm$, we obtain

$$\varphi_n^-(s,\rho) = \alpha(s)\rho\left(\frac{\eta_0(s)\,\check{\lambda}_n}{2\widehat{\tau}_0(s)} + \frac{\theta_n'(s)}{\eta_0(s)} + \frac{\widetilde{P}_n^-(s,\rho)}{\alpha(s)}\right)\mathsf{e}^-(s,\rho), \tag{B.1a}$$

$$\varphi_n^+(s,\rho) = \alpha(s)\rho\left(\frac{\eta_0(s)\,\check{\lambda}_n}{2\widehat{\tau}_0(s)} - \eta_0(s)\,\theta_n'(s) + \frac{\widetilde{P}_n^+(s,\rho)}{\alpha(s)}\right)\mathsf{e}^+(s,\rho). \tag{B.1b}$$

The first transmission condition $\varphi_n^-(\cdot,0) = \varphi_n^+(\cdot,0)$ is satisfied because $\varphi_n^\pm(\cdot,0) = 0$. Using the second transmission condition $-\eta_0^{-2}\,\partial_\rho\varphi_n^-(\cdot,0) = \partial_\rho\varphi_n^+(\cdot,0)$ and the expressions in Eq. (B.1), we get

$$-\eta_0^{-2}\left(\frac{\eta_0(s)\,\check{\lambda}_n}{2\widehat{\tau}_0(s)} + \frac{\theta_n'(s)}{\eta_0(s)} + \frac{\widetilde{P}_n^-(s,0)}{\alpha(s)}\right) = \frac{\eta_0(s)\,\check{\lambda}_n}{2\widehat{\tau}_0(s)} - \eta_0(s)\,\theta_n'(s) + \frac{\widetilde{P}_n^+(s,0)}{\alpha(s)}.$$

Solving for θ_n' and integrating yields

$$\theta_n(s) = \int_0^s \frac{\check{\lambda}_n}{2\widehat{\tau}_0(t)(1-\eta_0(t)^{-2})} + \frac{\eta_0(t)\widetilde{P}_n^-(t,0) + \eta_0(t)^3\widetilde{P}_n^+(t,0)}{\alpha(t)\,(\eta_0(t)^4 - 1)}\,\mathrm{d}t.$$

Now, the condition $\exp(\mathrm{i}\,h^{n-1}\,\theta_n) \in \mathscr{C}^\infty(\mathbb{T}_L)$ imposes $\theta_n(L) = \theta_n(0)$, solving for $\check{\lambda}_n$ and using the relation $\tau_0(t)^2\,(1-\eta_0^{-2}) = \varsigma$ yields

$$\check{\lambda}_n = -\frac{2\,\varsigma}{\langle\tau_0\rangle^2}\left\langle \frac{\eta_0\widetilde{P}_n^-(\cdot,0) + \eta_0^3\widetilde{P}_n^+(\cdot,0)}{\alpha\,(\eta_0^4-1)}\right\rangle.$$

Setting $P_n^\pm(s,\rho) = \alpha(s)\rho\left(\frac{\eta_0(s)\,\check{\lambda}_n}{2\widehat{\tau}_0(s)} \mp \eta_0(s)^{\pm 1}\theta_n'(s) + \frac{\widetilde{P}_n^\pm(s,\rho)}{\alpha(s)}\right)$ finishes the proof. □

B.3. Additional results for Schwartz functions.

Lemma B.1. *Consider* $F : (h; s, \rho) \mapsto F(h; s, \rho)$ *in* $\mathscr{C}^\infty([0, \frac{L}{2\pi}] \times \mathbb{T}_L, \mathscr{S}(\mathbb{R}_\pm))$, $\rho > 0$, *and the intervals* $I_-(h) = (-\infty, -\frac{\rho}{h})$ *and* $I_+(h) = (\frac{\rho}{h}, +\infty)$. *Then*

$$\int_{\mathbb{T}_L} \int_{I_\pm(h)} |F(h; s, \rho)|^2 \,\mathrm{d}\rho \,\mathrm{d}s = \mathcal{O}(h^\infty) \quad \text{as } h \to 0.$$

Proof. Notice that, for any integer $N \geq 1$, there exists a constant $C_N > 0$ such that $|\rho^N F(h; s, \rho)| \leq C_N$ for all $(h; s, \rho) \in [0, \frac{L}{2\pi}] \times \mathbb{T}_L \times \mathbb{R}_\pm$. Hence,

$$\int_{\mathbb{T}_L} \int_{I_\pm(h)} |F(h; s, \rho)|^2 \,\mathrm{d}\rho \,\mathrm{d}s \leq \frac{C_N\, L}{(2N-1)\, \rho^{2N-1}}\, h^{2N-1},$$

which finishes the proof. □

B.4. Additional results used in Section 4.

Lemma B.2. *For* $s \in \mathbb{T}_L$,

$$\theta_1(s) = \int_0^s \frac{\breve{\lambda}_1}{\breve{\lambda}_0} \widehat{\tau}_0(t) + \frac{(\eta_0(t)^2 - 1)\, \kappa(t)}{2\, \eta_0(t)} + \frac{\eta_1(t)}{2\, \eta_0(s)^2\, (\eta_0(t)^2 - 1)} + \mathrm{i}\, \frac{(\eta_0(t)^4 + 3)\, \eta_0'(t)}{2\, \eta_0(t)\, (\eta_0(t)^4 - 1)} + \mathrm{i}\, \frac{\alpha'(t)}{\alpha(t)} \,\mathrm{d}t.$$

Proof. This follows from the computation performed in Appendix B.2 where we solve Eq. (4.14) for $n = 1$ with

$$\begin{aligned} \eta_0^2 S_0^- &= 2\rho \frac{\eta_1}{\eta_0} \partial_\rho^2 \varphi_0^- - \left(\kappa - \frac{2\eta_1}{\eta_0}\right) \partial_\rho \varphi_0^- - 2\mathrm{i}\theta_0' \partial_s \varphi_0^- \\ &\quad - \left(2\rho {\theta_0'}^2 \left(\kappa + \frac{\eta_1}{\eta_0}\right) + \mathrm{i}\theta_0'' - 2\mathrm{i}\theta_0' \frac{\eta_0'}{\eta_0}\right) \varphi_0^-, \\ -S_0^+ &= -\kappa \partial_\rho \varphi_0^+ - 2\mathrm{i}\theta_0' \partial_s \varphi_0^+ - \left(2\rho {\theta_0'}^2 \kappa + \mathrm{i}\theta_0''\right) \varphi_0^+. \end{aligned}$$

□

Department of Applied Mathematics, University of California, Merced, 5200 North Lake Road, Merced, CA 95343, USA, Univ Lyon, INSA Lyon, UJM, UCBL, ECL, CNRS UMR 5208, ICJ, F-69621, France.
Email address: camille.carvalho@insa-lyon.fr

Karlsruhe Institute of Technology, Institute for Analysis, Englerstrasse 2, D-76131 Karlsruhe, Germany.
Email address: zois.moitier@kit.edu