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Perturbation of eigenvalues and scattering resonances with applications in imaging

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Abstract

English

This thesis contributes to the study of eigenvalue and scattering resonance perturbations caused by domain variations. We derive asymptotic formulae with layer potential techniques, and use them to image small particles.

We present several new results. We compute higher-order terms in the asymptotic expansions of eigenvalues, study their simplicity, and derive a variational characterization in the case of multiplicity higher than one. We report the results of different numerical experiments which validate and illustrate our findings, and propose computational techniques to reconstruct small domain variations from eigenvalue perturbations. We also study the asymptotic behavior of scattering resonances, first formally, via the method of matched expansions, and then rigorously, using the spectral properties of the Newtonian potential. We focus in particular on the analysis of plasmonic and highly refractive nanoparticles. Our formulae can be applied to the analysis and design of resonant structures.

Italiano

Questa tesi contribuisce allo studio di perturbazioni di autovalori e risonanze di scattering causate da variazioni di dominio. Deriviamo formule asintotiche con i potenziali di superficie, e le utilizziamo per ricostruire la forma di piccole particelle.

Presentiamo diversi risultati nuovi. Calcoliamo termini di grado superiore negli sviluppi asintotici degli autovalori, studiamo la loro semplicità, e deriviamo una caratterizzazione variazionale nel caso di molteplicità superiore a uno. Riferiamo i risultati di diversi esperimenti numerici che validano e illustrano le nostre conclusioni, e proponiamo tecniche computazionali per ricostruire piccole variazioni di domini da perturbazioni di autovalori. Studiamo anche il comportamento asintotico di risonanze di scattering, prima formalmente, attraverso il metodo delle espansioni

abbinate, e poi rigorosamente, utilizzando le proprietà spettrali del potenziale Newtoniano. In particolare ci focalizziamo sull'analisi di nano-particelle plasmoniche e altamente rifrangenti. Le nostre formule si possono applicare all'analisi e alla progettazione di strutture risonanti.

Introduction

In this thesis, we study the asymptotic behavior of eigenvalues and scattering resonances with respect to different types of domain perturbations. Our purpose is to develop some procedures to quickly estimate quantities of interest, and provide asymptotic error bounds.

The dependence of the spectrum of a differential operator on its domain of definition has been a thoroughly studied topic since the seminal work of Hadamard in the early 20th century. Probably even a larger literature has been devoted to the development of a perturbation theory for eigenvalues of linear operators, first from the quantum physics community, and then from the point of view of mathematical analysis. The foundational results of this area can be found in the works of Rellich and Kato from the mid 20th century. However, there is much interest in this line of research still today. For instance, the shift of eigenvalues caused by singular domain perturbations is a problem recently examined, with techniques from layer potential theory, by Ammari and collaborators. One of the goals of this thesis is an extension of these results. In fact, in Chapter 2, we show how the generalized argument principle of Gohberg and Sigal can be used to derive new higher-order terms in the asymptotic expansion of Neumann eigenvalues of the Laplacian.

A related issue, which has also been examined extensively in the literature, concerns the behavior of repeated eigenvalues. However, we believe that the study of repeated eigenvalues, for some particular operators, has not been thoroughly pursued, mainly due to the results of Uhlenbeck and Micheletti in the 60s and 70s, which state that, generically, eigenvalues are simple. We report these results in Chapter 3, where we also provide some generalizations to non-smooth domains and Neumann boundary conditions. One of the highlights of this thesis is a new variational characterization for multiple eigenvalues of self-adjoint, elliptic differential operators, presented in Chapter 4. We also discuss in Chapter 5 its applications to domain variations, which are of interest in applications.

A natural extension to the setting examined so far is to consider scattering resonances on unbounded domains. This is another area of research, rooted in the work on scattering theory by Lax and Phillips in the '60s, which is still active today, with recent results from Popov, Vodev, Zworski, and collaborators. Scattering resonances are of great importance in physics and technology, and new results in this setting are of great interest in applications, especially due to recent advancements in nano-optics and micro-biology. The mathematical models in these areas, however, often differ among communities and use fundamentally diverse assumptions and terminology. In this thesis, we provide a mathematical framework to analyze perturbations of scattering resonances, focusing our attention on scalar waves. We show how a modification of the scatterers influences the resonances, and derive new asymptotic expansions, first formally in Chapter 6 with the method of matching asymptotic expansions, and then rigorously in Chapter 7, using the spectral properties of the Newtonian potential and pole-pencil decompositions of the involved operator-valued functionals. We focus our attention on analyzing some situations which are currently of great interest in nano-opitcs: whispering gallery resonators, plasmonic nanoparticles, and finally, in Chapter 8, highly refractive particles. In all of these cases, we derive new asymptotic formulae, which can be used for the analysis and design of nano-structures with given resonance requirements.

We move on to present more in detail the topics of each chapter.

Structure of the thesis. The thesis is divided into eight chapters.

In Chapter 1, we fix the notation which will be used through the rest of the thesis and recall some useful results from the literature, mainly regarding Bessel functions, fundamental solutions, layer potentials and Gohberg-Sigal theory. We also describe the tools used to numerically validate the theoretical results.

In Chapter 2, we derive some terms in the small-volume asymptotic expansion of the shift of Neumann eigenvalues of the Laplacian caused by a grounded inclusion of area ε^2. We present a new higher-order explicit formula to compute them from the capacity, the eigenvalues and the eigenfunctions of the unperturbed domain, and the size and the position of the inclusion. The key step in the derivation is the filtering of the spectral decomposition of the Neumann function with the residue theorem. As a consequence of the formula, when a bifurcation of a double eigenvalue occurs (as for example in the case of a generic inclusion inside a disk) one eigenvalue decays like $O(1/\log\varepsilon)$, the other like $O(\varepsilon^2)$. The results of this chapter have been published in [38].

In Chapter 3, we construct an arbitrarily small and localized perturbation of any Lipschitz domain, which splits the Dirichlet, Neumann, or Robin repeated eigenvalues of the Laplacian into simple ones. We showcase two different approaches. The first one consists in the excision of a hole inside the domain and the perturbation of its boundary, and is based on a Hadamard's formula and sharp spectral stability estimates. The second one consists in the deformation of the boundary of the domain itself, and requires further properties of the bilinear form of the variational problem. The results of this chapter are the subject of [39].

In Chapter 4, we derive a new variational characterization for the shift of eigenvalues caused by a general type of perturbation for self-adjoint elliptic differential operators. This result allows the direct extension of asymptotic formulae from simple eigenvalues to repeated ones. It generalizes the results from Chapter 2 to higher multiplicity eigenvalues. Some interesting examples for the Laplacian are presented theoretically and numerically for the following domain perturbations: excision of a small hole, local change of conductivity, small boundary deformation. The results of this chapter are the subject of [40].

In Chapter 5, we present some techniques to reconstruct features of domain perturbations from the shift of eigenvalues they cause in a closed resonator. For this purpose, we use asymptotic formulae, under the assumption of smallness of the perturbations considered. The main appeal of the methods introduced is that they provide a very quick estimate of particles' features of any shape and in any dimension. We provide also many practical numerical examples, considering different types of perturbations. The results of this chapter are the subject of [44].

In Chapter 6, we derive formally a small-volume expansion for the scattering resonances of an open cavity perturbed by a small particle. We derive an asymptotic expression for the induced shift of the scattering frequencies, without neglecting the radiation effect. We consider also the case of plasmonic particles and show that they cause a stronger enhancement in the frequency shift. The derived formula can be used to image small particles located near the boundary of an open resonator which admits whispering-gallery modes. Numerical examples of interest for applications are also presented. The results of this chapter are the subject of [5].

In Chapter 7, we consider the transverse electric polarization case, and derive a small-volume formula for the shifts in the scattering resonances of a radiating dielectric cavity perturbed by small particles. We show that again a strong enhancement in the frequency shift appears in the case of plasmonic particles. We also consider exceptional scattering resonances and characterize their asymptotic behavior for a specific form of the Green's function. Our approach relies on pole-pencil decompositions of volume integral operators. The results of this chapter are the subject of [6].

In Chapter 8, we analyze the subwavelength resonances of dielectric particles with high refractive indices. We show that for an arbitrary shaped particle, these subwavelength resonances can be expressed in terms of the eigenvalues of the Newtonian potential associated with its shape. We derive an asymptotic estimate for the enhancement of the scattered field at the resonant frequencies. We also characterize the hybridization of the subwavelength resonances of a dimer of highly refractive dielectric nanoparticles. The results of this chapter are the subject of [7].

Chapter 1

Fundamental notation and results

In this chapter, we fix the notation and recall some results from the literature which will be extensively used through the rest of the thesis.

Reference space. We will mostly work with *domains*, which we define as subsets of $\mathbb{R}^d$ which are open, bounded, connected, and have Lipschitz boundaries. We reserve since now the symbol Ω to indicate such an arbitrary domain.

Basic notation. We collect here some notation and assumptions which will be used often.

- We assume any function and any set we work with to be Lebesgue measurable. We indicate with $|x|$ the modulus, the norm, or the Lebesgue measure of x, depending on x being a number, a vector, or a set.
- We indicate as ν the outward normal to a boundary $\partial\Omega$, as $\dfrac{\partial}{\partial\nu}$ or $\dfrac{\partial}{\partial\nu}\Big|_+$ the normal derivative from the exterior of Ω, and as $\dfrac{\partial}{\partial\nu}\Big|_-$ the normal derivative from the interior.
- We indicate as I the identity map or, when working on a finite dimensional vector space with a fixed basis, the identity matrix.

Function spaces. The spaces of functions we will encounter most often are: $\mathrm{C}^{k,\alpha}(\Omega)$, the space of functions with α-Hölderian kth derivative in Ω; $\mathrm{C}^k(\Omega)$ the space of functions with continuous kth derivative; $\mathrm{L}^p(\Omega)$, the space of p-integrable functions on Ω; $\mathrm{H}^s(\Omega)$, the subset of $\mathrm{L}^2(\Omega)$ whose distributional derivatives up to order s are also in $\mathrm{L}^2(\Omega)$; $\mathrm{H}^1_0(\Omega)$, the subset of $\mathrm{H}^1(\Omega)$ with trace zero.

Bessel functions. Let $\alpha, z \in \mathbb{C}$. Let us recall here some fundamental results on the canonical solutions to Bessel differential equation $z^2 f''(z) + zf'(z) + (z^2 - \alpha^2)f(z) = 0$. The Bessel function J_α of the first kind and order α can be defined, when α is not a negative integer, as

$$J_\alpha(z) = \left(\frac{z}{2}\right)^\alpha \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(k+\alpha+1)} \left(\frac{z}{2}\right)^{2k}, \tag{1.1}$$

where Γ indicates the Gamma function, that is $\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}dt$. The series in (1.1) converges on the whole $\mathbb{C}$. When α is a negative integer we define $J_\alpha = -J_{-\alpha}$.

The Bessel function Y_α of the second kind and order α can be defined, when α is not an integer, as

$$Y_\alpha(z) = \frac{J_\alpha(z)\cos(\pi\alpha) - J_{-\alpha}(z)}{\sin(\pi\alpha)},$$

and, when α is an integer, as the limit of Y_β as $\beta \to \alpha$. Both J_α and Y_α are analytic on $\mathbb{C} \setminus (-\infty, 0]$. For the particular case of $\alpha = 0$, we have that

$$Y_0(t) = \frac{2}{\pi} \sum_{n=0}^{\infty} (-1)^n \left(\frac{t^n}{2^n n!}\right)^2 \log(\eta_n t),$$

with $\log \eta_n = \text{Euler-Mascheroni constant} - \log 2 + \sum_{k=1}^n (1/k)$.

The Hankel function $H_\alpha^{(1)}$ of the first kind and order α can be defined as

$$H_\alpha^{(1)}(z) = J_\alpha(z) + \mathrm{i}Y_\alpha(z).$$

We refer to [2, Chapter 9] for further details.

Fundamental solutions. Let L be a linear differential operator on $\mathbb{R}^d$. A *fundamental solution*, or *Green function*, of L is a distribution Γ such that

$$L\Gamma(\cdot, z) = \delta_z,$$

where δ_z is the Dirac mass function concentrated in z and the equality is intended in the distributional sense (see, for instance, [91]).

When L is the Helmholtz operator, that is $L = \Delta + \omega^2$, we have an explicit expression for the fundamental solution via the Hankel function. For any $\omega \in \mathbb{C} \setminus (-\infty, 0]$, $r > 0$, we define

$$\Gamma_\omega(r) = -\frac{\mathrm{i}}{4} \left(\frac{\omega}{2\pi r}\right)^{\frac{d}{2}-1} H^{(1)}_{\frac{d}{2}-1}(\omega r), \tag{1.2}$$

and

$$\Gamma_0(r) = \begin{cases} \dfrac{r}{2} & \text{if } d = 1, \\[2ex] \dfrac{1}{2\pi} \log r & \text{if } d = 2, \\[2ex] \dfrac{1}{d(2-d)|S^{d-1}|r^{d-2}} & \text{if } d \geq 3, \end{cases} \tag{1.3}$$

where S^{d-1} is the $(d-1)$-dimensional unit sphere. We remark that our sign convention is the same as [48] but the opposite of [41].

When dealing with $x, z \in \mathbb{R}^d$, we define $\Gamma_\omega(x, z) = \Gamma_\omega(|x-z|)$. As a consequence of the definitions, Γ_ω is a fundamental solution for the operator $\Delta + \omega^2$ on $\mathbb{R}^d$ for any $\omega \in \mathbb{C} \setminus (-\infty, 0)$, that is

$$(\Delta_x + \omega^2)\Gamma_\omega(|x - z|) = \delta_z(x).$$

We remark that there is no guarantee of uniqueness for fundamental solutions. In fact, whenever working on a bounded domain, for simplicity we will substitute $\Gamma_\omega(r)$ with its real part, that is

$$\frac{1}{4}\left(\frac{\omega}{2\pi r}\right)^{\frac{d}{2}-1} Y_{\frac{d}{2}-1}(\omega r). \tag{1.4}$$

This simplifies the numerical computations and allows us to restrict the whole analysis to real numbers, since for bounded domains we will consider exclusively $\omega \in \mathbb{R}$. On unbounded domains, on the contrary, we must use $\Gamma_\omega(r)$ as defined in (1.2), due to the requirement of a radiation condition, which we now specify.

Sommerfeld radiation condition. A function $u : \mathbb{R}^d \to \mathbb{C}$, which is a solution to Helmholtz equation $(\Delta + \omega^2)u = 0$, satisfies the *Sommerfeld radiation condition* if

$$\frac{\partial u}{\partial \nu} - \mathrm{i}\omega u \to 0 \quad \text{in } \mathrm{L}^2(B_r) \quad \text{as } r \to \infty, \tag{1.5}$$

where B_r is the ball of radius r centered at the origin.

The physical meaning of the condition is to select the outgoing waves among all possible solutions to the Helmholtz problem. We remark that Γ_ω, as defined in (1.2), can be characterized as the unique fundamental solution which satisfies the Sommerfeld radiation when $\omega \in \mathbb{C} \setminus (-\infty, 0]$, and when $\omega = 0$, as the unique limit of $\Gamma_{\omega'}$ as $\omega' \to 0$.

Layer potentials. A fundamental tool which we will use extensively is that of boundary layer potentials, which we now introduce.

Definition 1.1. The *single layer potential*, the *double layer potential*, and the *Neumann-Poincaré operator* of Ω at frequency $\omega \in \mathbb{C} \setminus (-\infty, 0)$ are defined respectively as the operators $\mathcal{S}_\Omega^\omega$, $\mathcal{D}_\Omega^\omega$, $\mathcal{K}_\Omega^\omega$ such that for every $\phi \in \mathrm{L}^2(\partial\Omega)$ it holds

$$\mathcal{S}_\Omega^\omega[\phi](x) = \int_{\partial\Omega} \Gamma_\omega(|x-y|)\phi(y)\, d\sigma(y), \text{ for } x \in \mathbb{R}^d, \tag{1.6}$$

$$\mathcal{D}_\Omega^\omega[\phi](x) = \int_{\partial\Omega} \frac{\partial\Gamma_\omega(|x-y|)}{\partial\nu(y)}\phi(y)\, d\sigma(y), \text{ for } x \in \mathbb{R}^d \setminus \partial\Omega, \tag{1.7}$$

$$\mathcal{K}_\Omega^\omega[\phi](x) = \int_{\partial\Omega} \frac{\partial\Gamma_\omega(|x-y|)}{\partial\nu(y)}\phi(y)\, d\sigma(y), \text{ for } x \in \partial\Omega, \tag{1.8}$$

where the integral in (1.8) is intended to be in the principal value sense.

In the following propositions, we recall some properties of the layer potentials which we will need later.

Proposition 1.2. *The* L^2*-adjoint of* $\mathcal{K}_\Omega^{-\omega}$*, which we indicate as* $(\mathcal{K}_\Omega^\omega)^*$*, satisfies*

$$(\mathcal{K}_\Omega^\omega)^*[\phi](x) = \int_{\partial\Omega} \frac{\partial\Gamma_\omega(|x-y|)}{\partial\nu(x)}\phi(y)\, d\sigma(y), \text{ for } x \in \partial\Omega.$$

Moreover $\mathcal{K}_\Omega^\omega$ *is bounded from* $\mathrm{L}^2(\partial\Omega)$ *to* $\mathrm{H}^1(\partial\Omega)$*.*

Proposition 1.3. *The single layer potential,* $\mathcal{S}_\Omega$*, and the normal derivative of the double layer potential,* $\partial\mathcal{D}_\Omega/\partial\nu$*, are both continuous across* $\partial\Omega$*. The normal derivative of the single layer potential and the double layer potential are both discontinuous across* $\partial\Omega$ *and*

$$\left.\frac{\partial\mathcal{S}_\Omega^\omega}{\partial\nu}\right|_\pm = \pm I/2 + (\mathcal{K}_\Omega^\omega)^*, \tag{1.9}$$

$$\mathcal{D}_\Omega^\omega|_\pm = \mp I/2 + \mathcal{K}_\Omega^\omega. \tag{1.10}$$

For an in-depth study of the properties of layer potentials and their extensive applications in the theory of boundary value problems we refer to [35, 97].

Capacity of a set. The single layer potential can be used to define the capacity of a set, a useful quantity related to its geometry, as follows. It can be shown that there exists a unique non-zero couple $(\varphi_{\mathrm{cap}}, a) \in \mathrm{L}^2(\partial\Omega) \times \mathbb{R}$ which solves

$$\begin{cases} \mathcal{S}_\Omega^0[\varphi_{\mathrm{cap}}](x) \equiv a \quad \forall x \in \partial\Omega, \\ \int_{\partial\Omega} \varphi_{\mathrm{cap}} = 1. \end{cases}$$

Then the *capacity* of $\partial\Omega$ is defined as

$$\operatorname{cap}\partial\Omega = \begin{cases} e^{2\pi a} & \text{if } d = 2, \\ 1/a & \text{if } d \geq 2. \end{cases}$$

For further details on the capacity see [59, Section 16.4] and [25].

Polarization tensors. The *polarization tensor* $M(k,\Omega)$ of a domain Ω with coefficient $k \in \mathbb{C}$, is a $d \times d$ matrix which (i,j)-th entry is

$$\int_{\partial\Omega} \left(\frac{k+1}{2(k-1)} I - (\mathcal{K}_\Omega^0)^* \right)^{-1} (\nu_j) y_i \, d\sigma(y), \tag{1.11}$$

where ν_j, y_i indicate respectively the jth and ith components of ν and y.

The polarization tensor encodes different geometric properties of the underlying domain Ω. For the discussion of this result and many other properties we refer to [12]. We recall here only the fact that if Ω is a two dimensional ellipse with semi-axes a and b, rotated counter-clockwise by a degree α with respect to the coordinate axes, we can explicitly compute

$$M(k,\Omega) = (k-1) R_\alpha \begin{pmatrix} \dfrac{a+b}{a+kb} & 0 \\ 0 & \dfrac{a+b}{a+kb} \end{pmatrix} R_\alpha^T, \quad \text{with } R_\alpha = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}. \tag{1.12}$$

Gohberg-Sigal theory. Recall that if $f : \mathbb{C} \to \mathbb{C}$ is meromorphic, then the argument principle states that for any subset $V \subseteq \mathbb{C}$ with smooth boundary ∂V on which f has no poles and no zeros, it holds

$$\frac{1}{2\pi \mathrm{i}} \int_{\partial V} \frac{f'(z)}{f(z)} \, dz = N - P,$$

where N and P are respectively the number of zeros and poles of f inside V, counted with their multiplicity. An analogous result can be formulated for infinite dimensional operators. Its formulation however requires the introduction of some technical definitions, which we briefly summarize hereafter.

Let A be a functional from $\mathbb{C}$ to the space $\mathcal{L}$ of linear operators between two arbitrary Banach spaces. A point $z_0 \in \mathbb{C}$ is a *characteristic value* of A, if there exists a function $\phi(z)$ holomorphic and non-zero at z_0, and such that $A(z)\phi(z)$ is holomorphic and zero at z_0.

We say that A is *finitely meromorphic* at a point $z_0 \in \mathbb{C}$ which is a pole for A, if it can be written as

$$A(z) = \sum_{j \geq -s} (z - z_0)^j A_j,$$

for some natural number s, and if $A_{-1}, \dots, A_{-s}$ are finite dimensional operators. It is easy to show that if A is finitely meromorphic at z_0 then $\int_{\partial V} A(z)dz$ is a finite-dimensional operator for any V which contains no other poles than z_0.

Recall that an operator is called *Fredholm* if its kernel and cokernel are both finite dimensional. With these notions we can formulate a generalization of the argument principle as follows.

Theorem 1.4. *Let A be an operator-valued functional which is finitely meromorphic and Fredholm in V, continuous and invertible on ∂V. Then*

$$\frac{1}{2\pi \mathrm{i}} \operatorname{tr} \left(\int_{\partial V} A^{-1}(z) \partial_z A(z)\ dz \right) = N - P,$$

where N and P are respectively the number of characteristic values and of poles of $A(z)$ in V, counted with their multiplicities.

For the proof of this result and further details we refer to [49, 14].

Tools used for numerical validation. Various numerical experiments have been performed to validate the theoretical formulae obtained in this thesis. Finite element simulations for eigenvalue system have been performed with the `pdeeig` function from `MATLAB`. The predefined triangular mesh has been used, varying the number of recursive refinements until convergence of the required significant digits for each experiment.

The multipole expansion method has been implemented in `MATLAB` following the exposition of [73]. Although this method converges much faster than the finite element approach, it relies on summation formulae of elliptic functions, and is thus limited to problems where the shapes involved are ellipsoids.

Calculations of the terms appearing in the derived asymptotic formulae have been performed in `Mathematica`. To evaluate numerically the oscillatory integrals involved in the higher-order terms of some asymptotic formulae, the function `NIntegrate` with adaptive sampling has been used.

Chapter 2

Higher-order terms in a small volume expansion

Consider a planar bounded domain Ω and let ω^2 be an eigenvalue of the negative Laplacian on Ω with homogeneous Neumann boundary conditions. Suppose a small inclusion $D = z + \varepsilon B$ (where $z \in \Omega$, $|B| = |\Omega|$, and ε is small) is inserted inside Ω. This may cause the eigenvalue ω_ε^2 of the perturbed domain $\Omega \setminus D$ (with Neumann condition on $\partial\Omega$ and Dirichlet on ∂D) to vary in value or in multiplicity with respect to ω^2. Asymptotic formulae of the perturbation with respect to the size of the inclusion have been derived in the ‘80s in [86, 30]. In particular, it has been shown that if ω^2 is simple and u is the associated L^2-normalized eigenfunction, then the perturbation is singular and

$$\omega_\varepsilon^2 - \omega^2 = -\frac{2\pi|u(z)|^2}{\log\varepsilon} + o\left(1/\log(\varepsilon)\right). \tag{2.1}$$

More recently, Gohberg-Sigal theory for meromorphic operators applied to the integral equation formulation of the eigenvalue problem has led to new results (see [15, 22]). In this chapter we elaborate on these results to further improve (2.1), by calculating explicitly the terms up to $O(\varepsilon^2)$ and by generalizing it to the case of multiplicity 2. As a consequence of our derivation, for perturbed eigenvalues $\omega_{\varepsilon,1}^2 < \omega_{\varepsilon,2}^2$ splitted from a double eigenvalue ω^2 of the original domain Ω, it holds

$$\begin{aligned}
\omega_{\varepsilon,2} - \omega &= -\frac{C_1}{\log(\varepsilon) + C_2} + O(\varepsilon^2), \\
\omega_{\varepsilon,1} - \omega &= O(\varepsilon^2),
\end{aligned}$$

where C_1 and C_2 do not depend on ε and can be explicitly calculated from the capacity, the eigenvalues, and the value at z of the eigenfunctions of Ω.

This chapter is organized as follows. After introducing in Section 2.1 the precise setting of the problem and the notation, in Section 2.1.1 we recall the equivalent formulation of the Laplacian eigenvalues as characteristic values of an appropriate integral operator. An asymptotic expansion of this integral operator can be obtained by expanding in Taylor series the free space fundamental solution. Gohberg-Sigal theory then provides a link between eigenvalues' shifts and the traces of these integral operators through power sum polynomials. In Section 2.2, explicit terms for the small volume expansion of these power sum polynomials are derived by using properties of layer potentials. The key step in this derivation is the filtering of the spectral decomposition of the Neumann function using the residue theorem to obtain geometric-like series which can be summed. A proposal for formal automated computation of higher-order coefficients is given in Section 2.2.3. Finally in Section 2.3 some interesting consequences for special cases and a validation with numerical experiments are provided.

2.1 Preliminaries

The eigenvalue problem. Let Ω be an open, bounded and connected subset of $\mathbb{R}^2$ with C^1-boundary. It is well known that the eigenvalues of the negative Laplacian on Ω with Neumann boundary condition are non-negative, have finite multiplicity and can be arranged in an increasing divergent sequence

$$0 = \omega_0^2 < \omega_1^2 < \omega_2^2 < \cdots < \omega_k^2 \to \infty.$$

For each index i, let m_i be the multiplicity of ω_i^2. We choose the associated eigenfunctions $u_{i,1}, \ldots, u_{i,m_i}$ to be orthonormal in L^2. Thus, for any i, j, we have

$$\begin{cases} (\Delta + \omega_i^2) u_{i,j} = 0 & \text{in } \Omega, \\ \dfrac{\partial u_{i,j}}{\partial \nu} = 0 & \text{on } \partial\Omega, \end{cases}$$

and

$$\int_\Omega u_{i,j} u_{k,l} = \begin{cases} 1 & \text{if } i = k \text{ and } j = l, \\ 0 & \text{otherwise.} \end{cases}$$

We will often use the vector notation

$$U_i := (u_{i,1}, \ldots, u_{i,m_i}). \tag{2.2}$$

Invertibility of the single layer potential. Consider the special case when Ω is the unit disk. Writing t for the angle in the usual polar parametrization of the boundary, one can calculate that

$$\mathcal{S}_\Omega^0[e^{int}](\tau) = \begin{cases} 0 & \text{if } n = 0, \\ -\dfrac{1}{2n} e^{in\tau} & \text{otherwise.} \end{cases}$$

Thus, we have an explicit expression of $\mathcal{S}_\Omega^0$ in the Fourier basis of $\mathrm{L}^2(\partial\Omega)$. Notice however that the fact that $\mathcal{S}_\Omega^0[1] = 0$ causes the non-invertibilty of $\mathcal{S}_\Omega^0$. Nonetheless, if we consider

$$\phi \mapsto \mathcal{S}_\Omega^0[\phi] + \lambda \int_{\partial\Omega} \phi, \tag{2.3}$$

we see that, for a constant $\lambda \neq a$, this operator is always invertible from $\mathrm{L}^2(\partial\Omega)$ to $\mathrm{H}^1(\partial\Omega)$. This is still true for a more general domain Ω as in our assumptions (see [97, Theorem 4.11] for more details).

Fundamental solution for a bounded domain. The Neumann function N_Ω^ω is defined as the solution of

$$\begin{cases} (\Delta_x + \omega^2) N_\Omega^\omega(x, z) = \delta_z(x) & \text{for } x \in \Omega, \\ \dfrac{\partial N_\Omega^\omega(x, z)}{\partial \nu(x)} = 0 & \text{for } x \in \partial\Omega, \end{cases}$$

where $\omega \in \mathbb{C}$ is not one of ω_i and $z \in \Omega$. It has the spectral representation

$$N_\Omega^\omega(x, z) = \sum_{j=1}^{\infty} \frac{U_j(x) \cdot U_j(z)}{\omega^2 - \omega_j^2},$$

where the convergence of the series to N_Ω^ω in general is only in L^2 (see [37, *expansion theorems*]). Here, U_j is defined by (2.2).

By integrating N_Ω^ω against test functions in $\mathrm{L}^2(\partial\Omega)$ and using the properties of layer potentials one can show that

$$(I/2 - \mathcal{K}_\Omega^\omega)^{-1} [\Gamma_\omega(\,\cdot\,, z)](x) = N_\Omega^\omega(x, z). \tag{2.4}$$

We also recall that the Neumann function has a logarithmic singularity. In fact,

$$N_\Omega^\omega(x, z) = \frac{1}{2\pi} \log|x - z| + R_\Omega^\omega(x, z) \quad \forall x \neq z, \tag{2.5}$$

with R_Ω^ω being continuous on $\Omega \times \Omega$ (for more details on the last two results, see [14, Section 2.3.5] and the references therein).

The perturbed eigenvalue problem. Let B be a bounded domain with piecewise smooth boundary, with area $|B| = |\Omega|$, and centered at the origin in the sense that

$$\int_{\partial B} y_1 \, d\sigma(y_1, y_2) = \int_{\partial B} y_2 \, d\sigma(y_1, y_2) = 0.$$

We fix for the rest of the chapter a point $z \in \Omega$, a scaling factor $0 < \varepsilon \ll 1$ and an index $\theta \in \mathbb{N}$. Suppose then that the domain Ω is perturbed by inserting a grounded inclusion $D = z + \varepsilon B$ inside Ω. This causes the eigenvalue ω_θ^2 to split into m_θ (possibly distinct) eigenvalues $\omega_{\varepsilon,1}^2 \leq \cdots \leq \omega_{\varepsilon,m_\theta}^2$ with associated eigenfunctions $u_{\varepsilon,1}, \ldots, u_{\varepsilon,m_\theta}$. This means that for $j = 1, \ldots, m_\theta$,

$$\begin{cases} (\Delta + \omega_{\varepsilon,j}^2) u_{\varepsilon,j} = 0 & \text{in } \Omega \setminus D, \\ u_{\varepsilon,j} = 0 & \text{on } \partial D, \\ \dfrac{\partial u_{\varepsilon,j}}{\partial \nu} = 0 & \text{on } \partial \Omega. \end{cases}$$

It has been shown in [89] that under our assumptions $\omega_{\varepsilon,j}^2 \to \omega_\theta^2$ as $\varepsilon \to 0$. The problem we will consider is the following:

$$\text{to find an asymptotic expansion of } \omega_{\varepsilon,j}^2 - \omega_\theta^2 \text{ in terms of } \varepsilon, \text{ for all } j \in \{1, \ldots, m_\theta\}.$$

With this purpose, we will transform the eigenvalue problem into an equivalent integral formulation.

Nonstandard notation. In this chapter we will use the following notation:

- we indicate as $\displaystyle\oint$ the normalized complex path integral $\displaystyle\frac{1}{2\pi \mathrm{i}} \int$;
- for clarity, we adopt the symbol $\diamond$ to indicate the function variable of an operator evaluated at a point, e.g. $\mathcal{D}_\Omega^\omega[\diamond](z)$ indicates the function $\mathrm{L}^2(\partial\Omega) \ni \varphi \mapsto \mathcal{D}_\Omega^\omega[\varphi](z) \in \mathbb{R}$;
- given a multi-index $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d$ we indicate as ∂^α the normalized differential operator
$$\frac{1}{\alpha_1! \ldots \alpha_n!} \frac{\partial}{\partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d}}.$$

2.1.1 Integral formulation

Define $\mathcal{A}_\varepsilon(\omega)$ as

$$\mathbb{C} \ni \omega \quad \mapsto \quad \mathcal{A}_\varepsilon(\omega) = \begin{pmatrix} I/2 - \mathcal{K}_\Omega^\omega & -\mathcal{S}_D^\omega \\ & \\ \mathcal{D}_\Omega^\omega & \mathcal{S}_D^\omega \end{pmatrix},$$

meaning that for any fixed $\omega \in \mathbb{C}$, $\mathcal{A}_\varepsilon(\omega)$ is the operator which takes $\phi \in \mathrm{L}^2(\partial\Omega)$, $\psi \in \mathrm{L}^2(\partial D)$ to

$$\begin{pmatrix} (I/2 - \mathcal{K}_\Omega^\omega)[\phi] - \mathcal{S}_D^\omega[\psi] \\ \\ \mathcal{D}_\Omega^\omega[\phi] + \mathcal{S}_D^\omega[\psi] \end{pmatrix} \quad \in \quad \begin{matrix} \mathrm{L}^2(\partial\Omega) \\ \times \\ \mathrm{L}^2(\partial D). \end{matrix}$$

By expanding the fundamental solution in Taylor series in ε, one can show that $\mathcal{A}_\varepsilon$ has the same characteristic values as the operator $\sum_{n=0}^\infty \varepsilon^n \mathcal{H}_n$ (the series converges in operator norm), where

$$\mathcal{H}_0 = \begin{pmatrix} I/2 - \mathcal{K}_\Omega^\omega & -\Gamma_\omega(x,z)\int_{\partial B} \diamond(y)\, d\sigma(y) \\ & \\ \mathcal{D}_\Omega^\omega[\diamond](z) & \tilde{\mathcal{S}}_B^\omega \end{pmatrix},$$

$$\mathcal{H}_n = \begin{pmatrix} 0 & (-1)^{n+1}\sum_{|\alpha|=n} (\partial^\alpha \Gamma_\omega)(x,z)\int_{\partial B} y^\alpha \diamond(y)\, d\sigma(y) \\ & \\ \sum_{|\alpha|=n} (\partial^\alpha \mathcal{D}_\Omega^\omega[\diamond])(z) x^\alpha & \mathcal{X}_n \end{pmatrix},$$

with

$$\mathcal{X}_n = \begin{cases} \dfrac{\omega^n}{2^{n+1} n! \pi} \displaystyle\int_{\partial B} \log(\eta_{\frac{n}{2}} \omega\varepsilon|x-y|)|x-y|^n \diamond(y)\, d\sigma(y) & n \text{ even}, \\ \\ 0 & n \text{ odd}, \end{cases}$$

$$\tilde{\mathcal{S}}_B^\omega = \frac{1}{2\pi}\int_{\partial B} \log(\eta_0 \omega\varepsilon|x-y|) \diamond(y)\, d\sigma(y). \tag{2.6}$$

A study of the properties of A_ε can be found in [14, Chapter 1 and Section 3.1]). In the next proposition we collect only the properties which will be used in the following discussion. Recall that $\omega \in \mathbb{C}$ is a characteristic value of A_ε if the null-space of $A_\varepsilon(\omega)$ contains some non-zero function.

Proposition 2.1. *The following results hold:*

(i) $\omega \mapsto \mathcal{A}_\varepsilon(\omega)$ *is analytic on* $\mathbb{C} \setminus (-\infty, 0)$ *and* $\omega \mapsto \mathcal{A}_\varepsilon(\omega)^{-1}$ *is meromorphic in* $\mathbb{C}$*;*

(ii) ω_θ *is a characteristic value of* $I/2 - \mathcal{K}_\Omega^\omega$ *and a simple pole of* $(I/2 - \mathcal{K}_\Omega^\omega)^{-1}$*;*

(iii) $(\omega_{\varepsilon,j})_{j=1,\dots,m_\theta}$ *are characteristic values of* $\mathcal{A}_\varepsilon$*;*

(iv) *There is an open neighbourhood V (which we fix for the rest of the chapter) of ω_θ such that $\omega_{\varepsilon,j} \in V$ for $j = 1, \dots, m_\theta$, and no other characteristic values of $\mathcal{A}_\varepsilon$ are in V.*

Consider now the power sum polynomials

$$p_l = \sum_{j=1}^{m_\theta} (\omega_{\varepsilon,j} - \omega_\theta)^l.$$

By properties of symmetric polynomials we can express $\omega_{\varepsilon,1} - \omega_\theta$, $\dots$, $\omega_{\varepsilon,m_\theta} - \omega_\theta$ as roots of a polynomial $z^{m_\theta} + c_1 z^{m_\theta - 1} + \cdots + c_{m_\theta}$, where the coefficients c_k are themselves polynomials in p_j; in particular, the coefficients c_k can be recovered from the recurrence relations

$$p_{l+m_\theta} + c_1 p_{l+m_\theta-1} + \cdots + c_{m_\theta} p_l \qquad \text{for } l = 0, \dots, m_\theta - 1.$$

Example 2.2. If $m_\theta = 1$, we have

$$\omega_{\varepsilon,1} - \omega_\theta = p_1,$$

while if $m_\theta = 2$, then

$$\omega_{\varepsilon,2} - \omega_\theta = \frac{p_1 + \sqrt{2p_2 - p_1^2}}{2}, \qquad \omega_{\varepsilon,1} - \omega_\theta = \frac{p_1 - \sqrt{2p_2 - p_1^2}}{2}.$$

Hence, we have reduced the problem of finding an asymptotic expansion of $\omega_{\varepsilon,j}^2 - \omega_\theta^2$ to finding an asymptotic expansion of p_l. Before computing the explicit terms in the expansion of p_l we recall some crucial concepts from Gohberg-Sigal theory.

If A is a finite range operator on a Banach space, its trace $\operatorname{tr} A$ can be defined as the trace of A restricted to the finite dimensional space where A is non zero. In the next proposition we recall some properties of the trace which will be extensively used in the subsequent computations.

Proposition 2.3. *The following results hold:*

(i) *Suppose A_1, A_2, A_3, A_4 are finite dimensional operators on a Banach space. Then*

$$\operatorname{tr} \begin{pmatrix} A_1 & A_2 \\ A_3 & A_4 \end{pmatrix} = \operatorname{tr} A_1 + \operatorname{tr} A_4.$$

(ii) *Suppose B, C are operator valued maps defined on U, a neighborhood of a common singularity $\nu \in \mathbb{C}$. If B, C are analytic in $U \setminus \nu$ and have only finite* *dimensional operators in the negative terms of their Laurent expansion in ν, then $\int_{\partial U} B(\omega)C(\omega)\,d\omega$ is finite dimensional and*

$$\operatorname{tr}\oint_{\partial U} B(\omega)C(\omega)\,d\omega = \operatorname{tr}\oint_{\partial U} C(\omega)B(\omega)\,d\omega.$$

(iii) If P_ω is a projection from L^2 to $\mathbb{C}$ and $f_\omega \in \mathrm{L}^2$, then

$$\operatorname{tr}\oint_{\partial V} f_\omega P_\omega\,d\omega = \oint_{\partial V} P_\omega[f_\omega]\,d\omega.$$

An application of the argument principle for operator valued maps (Theorem 1.4) leads to the following crucial representation.

Theorem 2.4. *We can rewrite p_l as*

$$\begin{aligned} p_l = \; & \operatorname{tr}\oint_{\partial V} (\omega-\omega_\theta)^l \mathcal{H}_0(\omega)^{-1}\partial_\omega \mathcal{H}_0(\omega)\,d\omega \\ & + l\sum_{n=1}^{\infty}\varepsilon^n \sum_{j=1}^{n}\frac{(-1)^j}{j}\operatorname{tr}\oint_{\partial V}(\omega-\omega_\theta)^{l-1}\left(\sum_{\substack{n_1+\cdots+n_j=n\\ n_i\in\mathbb{Z}^+}}\prod_{k=1}^{j}\mathcal{H}_0(\omega)^{-1}\mathcal{H}_{n_k}(\omega)\right)d\omega. \end{aligned}$$

The previous expression can be obtained by following the same algebraic manipulations as those in the proof of [14, Theorem 3.9].

2.2 Computations for explicit formulae

First we highlight the quantities playing a key role in the expansion of p_l in the following definition.

Definition 2.5. Let α, β be multi-indices in $\mathbb{N}^2$. The *generalized capacity* of B of order (α,β), at frequency ω is

$$\mathfrak{c}_{\alpha,\beta}(\omega) = -\int_{\partial B}(\tilde{\mathcal{S}}_B^\omega)^{-1}[\xi^\alpha](y)\,y^\beta\,d\sigma(y),$$

where $\tilde{\mathcal{S}}_B^\omega$ is defined in (2.6). We also introduce

$$\mathfrak{t}(\omega) = \frac{U_\theta(z)\cdot\mathcal{D}_\Omega^\omega[U_\theta](z)}{\omega+\omega_\theta}, \qquad \mathfrak{r}(\omega) = \sum_{\substack{j=1\\ j\neq\theta}}^{\infty}\frac{U_j(z)\cdot\mathcal{D}_\Omega^\omega[U_j](z)}{\omega^2-\omega_j^2}, \tag{2.7}$$

where U_j is the vector of eigenfunctions associated to ω_j^2, as defined in (2.2).

In the subsequent discussion, we will often indicate the generalized capacity of order $(\alpha,0)$ as $\mathfrak{c}_\alpha$ instead of $\mathfrak{c}_{\alpha,0}$.

Remark 2.6. We collect some useful properties of the quantities introduced in the previous definition:

(i) The generalized capacity of order zero can be rewritten as

$$\mathfrak{c}_0(\omega) = -\int_{\partial B} (\tilde{\mathcal{S}}_B^\omega)^{-1}[1] = -\frac{2\pi}{\log(\eta_0 \omega \varepsilon \operatorname{cap} \partial B)}.$$

(ii) It holds $\mathfrak{c}_{\alpha,\beta} = 0$ if $|\alpha| + |\beta|$ is odd. This is a consequence of the fact that φ is even/odd if and only if $\mathcal{S}_B^0[\varphi]$ is even/odd (as functions parametrized on ∂B).

(iii) Although the series defining $\mathfrak{r}$ in (2.7) does not converge absolutely, Weyl's law (which states that $\omega_j^2 \sim j$) and the oscillatory nature of the eigenfunctions of Ω evaluated at z suggest that the series converges conditionally.

(iv) By exploiting the spectral expansion of the Neumann function (2.5), we have that

$$\mathcal{D}_\Omega^\omega[N_\Omega^\omega(\cdot, z)](z) = \frac{\mathfrak{t}(\omega)}{\omega - \omega_\theta} + \mathfrak{r}(\omega). \tag{2.8}$$

In the subsequent calculations, this identity will enable us to rewrite the expansion in Theorem 2.4 in terms of $\mathfrak{t}(\omega_\theta)$ and $\mathfrak{r}(\omega_\theta)$.

(v) By Green's identity and the defining property of Γ_{ω_θ} and U_θ, we can compute the special value

$$\mathfrak{t}(\omega_\theta) = \frac{|U_\theta(z)|^2}{2\omega_\theta}. \tag{2.9}$$

2.2.1 Zero-order term

Lemma 2.7. *The zero-order term in the expansion in powers of ε of p_l is*

$$\left(\frac{\mathfrak{t}(\omega_\theta)}{1/\mathfrak{c}_0(\omega_\theta) - \mathfrak{r}(\omega_\theta)} \right)^l. \tag{2.10}$$

Proof. By Theorem 2.4, our problem reduces to compute explicitly

$$\operatorname{tr} \oint_{\partial V} (\omega - \omega_\theta)^l \mathcal{H}_0(\omega)^{-1} \partial_\omega \mathcal{H}_0(\omega)\, d\omega.$$

To make further computations clearer and more concise, we rename

$$\begin{aligned} A &= I/2 - \mathcal{K}_\Omega^\omega[\diamond](x), & \Gamma &= \Gamma_\omega(x,z), \\ N &= N_\Omega^\omega(x,z), & D &= \mathcal{D}_\Omega^\omega[\diamond](z), \\ \mathfrak{s} &= \omega - \omega_\theta. \end{aligned} \tag{2.11}$$

The characteristic values of $\mathcal{H}_0$ are the $\omega \in \mathbb{C}$ for which there exist $\phi \in \mathrm{L}^2(\Omega), \psi \in \mathrm{L}^2(B)$, at least one of them non-zero, such that

$$\begin{cases} A\phi - \Gamma \int_{\partial B} \psi = 0, \\ D\phi + \tilde{\mathcal{S}}_B^\omega \psi = 0. \end{cases}$$

By recalling from (2.3) that $\tilde{\mathcal{S}}_B^\omega$ is invertible, applying $(\tilde{\mathcal{S}}_B^\omega)^{-1}$ and integrating the second equation of the system, we obtain

$$\int_{\partial B} \psi = \mathfrak{c}_0 D\phi.$$

Substituting this back into the first equation, we have that the characteristic values of the system correspond to the characteristic values of the operator

$$H = A - \mathfrak{c}_0 \Gamma D.$$

Therefore, the coefficient we are looking for will be given by

$$E = \operatorname{tr} \oint_{\partial V} \mathfrak{s}^l H^{-1} H' \, d\omega,$$

where $'$ denotes differentiation with respect to ω. A straightforward calculation shows that

$$H^{-1} = (I - \mathfrak{c}_0 ND)^{-1} A^{-1} = \sum_{m=0}^{\infty} (\mathfrak{c}_0 ND)^m A^{-1},$$

(where the m exponent indicates m times the composition of $c_0 ND$) and

$$H' = A' - \Gamma' \mathfrak{c}_0 D - \Gamma (\mathfrak{c}_0 D)'.$$

Then

$$H^{-1}H' = A^{-1}A' + \sum_{m=1}^{\infty} (\mathfrak{c}_0 ND)^m A^{-1} A' - (\mathfrak{c}_0 ND)^{m-1} A^{-1} \Gamma' \mathfrak{c}_0 D - (\mathfrak{c}_0 ND)^{m-1} N (\mathfrak{c}_0 D)'.$$

Since A is analytic in V, A^{-1} has a simple pole at ω_θ, and we are only interested in the case $l \geq 1$. Hence, we have

$$\oint_{\partial V} \mathfrak{s}^l A^{-1} A' = 0.$$

Then, by Item iii of Proposition 2.3,

$$E = \sum_{m=1}^{\infty} \operatorname{tr} \oint_{\partial V} \mathfrak{s}^l \left((\mathfrak{c}_0 ND)^m A^{-1} A' - N^{m-1} (\mathfrak{c}_0 D)^m A^{-1} \Gamma' - N^m (\mathfrak{c}_0 D)^{m-1} (\mathfrak{c}_0 D)' \right)$$

$$= \sum_{m=1}^{\infty} \oint_{\partial V} \mathfrak{s}^l \left(\mathfrak{c}_0^m (DN)^{m-1} D A^{-1} A' A^{-1} \Gamma - \mathfrak{c}_0^m (DN)^{m-1} D A^{-1} \Gamma' - (\mathfrak{c}_0 DN)^{m-1} (\mathfrak{c}_0 D)' N \right).$$

Since $(A^{-1})' = -A^{-1}A'A^{-1}$, by applying multiple times the chain rule, we arrive at

$$E = -\sum_{m=1}^{\infty} \frac{1}{m} \oint_{\partial V} \mathfrak{s}^l \left((\mathfrak{c}_0 DN)^m \right)'.$$

Then, by an integration by parts followed by a binomial expansion of $(DN)^m$, we have that

$$\begin{aligned} E &= \sum_{m=1}^{\infty} \frac{l}{m} \oint_{\partial V} \mathfrak{s}^{l-1} (\mathfrak{c}_0 DN)^m \\ &= \sum_{m=1}^{\infty} \frac{l}{m} \oint_{\partial V} \mathfrak{s}^{l-1} \mathfrak{c}_0^m \left(\frac{\mathfrak{t}}{\mathfrak{s}} + \mathfrak{r} \right)^m \\ &= \sum_{m=1}^{\infty} \frac{l}{m} \sum_{k=0}^{m} \binom{m}{k} \oint_{\partial V} \frac{1}{\mathfrak{s}^{k-l+1}} \mathfrak{c}_0^m \mathfrak{t}^k \mathfrak{r}^{m-k}. \end{aligned} \tag{2.12}$$

Since the only pole in V of the integrand is ω_θ, by applying the residue theorem we can cancel each addend of the sum on k except the one corresponding to a pole of order 1, obtaining

$$E = l\mathfrak{t}(\omega_\theta)^l \mathfrak{r}(\omega_\theta)^{-l} \sum_{m=l}^{\infty} \frac{1}{m} \binom{m}{l} (\mathfrak{c}_0(\omega_\theta)\mathfrak{r}(\omega_\theta))^m.$$

A final application of the identity

$$\sum_{m=l}^{\infty} \frac{1}{m} \binom{m}{l} x^m = \frac{1}{l} \left(\frac{x}{1-x} \right)^l,$$

leads to (2.10).

□

2.2.2 First-order term

Lemma 2.8. *The coefficient of the ε term in the expansion of p_l is zero.*

Proof. With the notation introduced in (2.11),

$$\mathcal{H}_1 = \sum_{|\alpha|=1} \begin{pmatrix} 0 & (\partial^\alpha \Gamma) \int_{\partial B} y^\alpha \diamond \\ (\partial^\alpha D) x^\alpha & 0 \end{pmatrix}.$$

By applying the blockwise inversion formula,

$$\begin{pmatrix} W & X \\ Y & Z \end{pmatrix}^{-1} = \begin{pmatrix} (W - XZ^{-1}Y)^{-1} & -W^{-1}X(Z - YW^{-1}X)^{-1} \\ -Z^{-1}Y(W - XZ^{-1}Y)^{-1} & (Z - YW^{-1}X)^{-1} \end{pmatrix},$$

to calculate $\mathcal{H}_0^{-1}$, and rewriting the inverses of sums of operators in a Neumann series, we obtain

$$\mathcal{H}_0^{-1} = \begin{pmatrix} (Nc_0 D)^m A^{-1} & N \int_{\partial B} (-(\tilde{\mathcal{S}}_B^\omega)^{-1}[1] DN \int_{\partial B})^m (\tilde{\mathcal{S}}_B^\omega)^{-1} \\ -(\tilde{\mathcal{S}}_B^\omega)^{-1}[1] D (Nc_0 D)^m A^{-1} & (-(\tilde{\mathcal{S}}_B^\omega)^{-1}[1] DN \int_{\partial B})^m (\tilde{\mathcal{S}}_B^\omega)^{-1} \end{pmatrix}.$$

A straightforward computation leads to

$$\mathcal{H}_0^{-1}\mathcal{H}_1 = \sum_{m=0}^{\infty} \sum_{|\alpha|=1} \begin{pmatrix} \mathfrak{c}_\alpha(...) & (...) \\ (...) & -(\tilde{\mathcal{S}}_B^\omega)^{-1}[1](...) \int_{\partial B} y^\alpha \diamond \end{pmatrix},$$

where we omit most of the terms by writing (...) instead. They indeed do not count towards our calculations, since from the fact that $\mathfrak{c}_\alpha = 0$ for $|\alpha| = 1$, we have that the coefficient of ε is

$$\operatorname{tr} \oint_{\partial V} \mathfrak{s}^{l-1} \mathcal{H}_0^{-1}\mathcal{H}_1 = \operatorname{tr} \oint_{\partial V} \mathfrak{s}^{l-1} \left((\mathcal{H}_0^{-1}\mathcal{H}_1)_{11} + (\mathcal{H}_0^{-1}\mathcal{H}_1)_{22} \right) = \mathfrak{c}_\alpha(\dots) = 0.$$

□

2.2.3 On higher-order terms

In this subsection we propose a method to calculate explicitly any coefficient of the expansion of p_l. To the shorthand notation introduced in (2.11) we add $a = DN$, $S = \tilde{\mathcal{S}}_B^\omega$, $\phi = -S^{-1}[1]$. Then, we can rewrite

$$\mathcal{H}_0^{-1} = \begin{pmatrix} A^{-1} & N \int_{\partial B} S^{-1} \\ \phi D A^{-1} & S^{-1} \end{pmatrix} + \sum_{m=1}^{\infty} \begin{pmatrix} N \mathfrak{c}_0^m a^{m-1} D A^{-1} & N(\mathfrak{c}_0 a)^m \int_{\partial B} S^{-1} \\ \phi(\mathfrak{c}_0 a)^m D A^{-1} & \phi \mathfrak{c}_0^{m-1} a^m \int_{\partial B} S^{-1} \end{pmatrix},$$

and

$$\mathcal{H}_n = \sum_{|\alpha|=n} \begin{pmatrix} 0 & (-1)^{n+1} (\partial^\alpha \Gamma) \int_{\partial B} y^\alpha \diamond (y)\, d\sigma(y) \\ (\partial^\alpha D) x^\alpha & \mathcal{X}_n \end{pmatrix}.$$

An explicit computation leads to

$$-\mathcal{H}_0^{-1}\mathcal{H}_n = \sum_{|\alpha|=n} \begin{pmatrix} N c_\alpha \partial^\alpha D & (-1)^n A^{-1} \partial^\alpha \Gamma \int_{\partial B} y^\alpha \diamond - N \int_{\partial B} S^{-1} \mathcal{X}_n \\ c_\alpha \partial^\alpha D & (-1)^n \phi D A^{-1} \partial^\alpha \Gamma \int_{\partial B} y^\alpha \diamond - S^{-1} \mathcal{X}_n \end{pmatrix}$$

$$+ \sum_{m=1}^{\infty} \begin{pmatrix} N(\mathfrak{c}_0 a)^m \mathfrak{c}_\alpha \partial^\alpha D & (-1)^n N \mathfrak{c}_0^m a^{m-1} D A^{-1} (\partial^\alpha \Gamma) \int_{\partial B} y^\alpha \diamond - N(\mathfrak{c}_0 a)^m \int_{\partial B} S^{-1} \mathcal{X}_n \\ \phi \mathfrak{c}_0^{m-1} a^m \mathfrak{c}_\alpha \partial^\alpha D & (-1)^n \phi (\mathfrak{c}_0 a)^m D A^{-1} (\partial^\alpha \Gamma) \int_{\partial B} y^\alpha \diamond - \phi \mathfrak{c}_0^{m-1} a^m \int_{\partial B} S^{-1} \mathcal{X}_n \end{pmatrix}.$$

Since all elements of the matrix are one-dimensional projection operators on either N, ϕ or 1, the operator $-\mathcal{H}_0^{-1}\mathcal{H}_n$ has the same characteristic values of the projection operator on 1 given by

$$\sum_{|\alpha|=n}\begin{pmatrix} c_\alpha(\partial^\alpha D)N & (-1)^n \int_{\partial B} y^\alpha A^{-1}\partial^\alpha\Gamma - \int_{\partial B} S^{-1}\mathcal{X}_n N \\ c_\alpha(\partial^\alpha D)[1] & (-1)^n \mathfrak{c}_{0,\alpha} DA^{-1}\partial^\alpha\Gamma - S^{-1}\mathcal{X}_n[1] \end{pmatrix}$$

$$+\sum_{m=1}^{\infty}\begin{pmatrix} (\mathfrak{c}_0 a)^m \mathfrak{c}_\alpha(\partial^\alpha D)N & (-1)^n \mathfrak{c}_0^m a^{m-1} DA^{-1}(\partial^\alpha\Gamma)\int_{\partial B} y^\alpha N - (\mathfrak{c}_0 a)^m \int_{\partial B} S^{-1}\mathcal{X}_n N \\ \mathfrak{c}_0^{m-1} a^m \mathfrak{c}_\alpha(\partial^\alpha D)\phi & (-1)^n(\mathfrak{c}_0 a)^m DA^{-1}(\partial^\alpha\Gamma)\mathfrak{c}_{0,\alpha} - \mathfrak{c}_0^{m-1} a^m \int_{\partial B} S^{-1}\mathcal{X}_n\phi \end{pmatrix}. \tag{2.13}$$

Suppose that the elements of the matrices in (2.13) can be rewritten explicitly in terms of sums of powers of the singularity $\mathfrak{s}$. The same approach used to derive the zero-order term in the previous section could then be applied to compute explicitly

$$\operatorname{tr}\oint_{\partial V} \mathfrak{s}^{l-1}\mathcal{H}_0^{-1}\mathcal{H}_{n_1}\dots\mathcal{H}_0^{-1}\mathcal{H}_{n_j}.$$

Substituting this value back in the expression for p_l in Theorem 2.4, we could compute, for example with the aid of a computer algebra system, any of the coefficients of the expansion in ε.

However, the task of rewriting explicitly the singularity $\mathfrak{s}$ in (2.13) for $\alpha \geq 1$ is not trivial, as identities similar to (2.4) and (2.8), but involving the terms $(\partial^\alpha D)N$, $A^{-1}\partial^\alpha\Gamma$ and $S^{-1}\mathcal{X}_n N$ would need to be determined.

2.3 Results for special cases

We collect in this final section some interesting results which follow directly, or with minor algebraic manipulations, from Lemmas 2.7, 2.8, and Example 2.2.

Proposition 2.9. *Suppose that ω_θ is simple.*

(i) We have

$$\omega_{\varepsilon,1} - \omega_\theta = \frac{\mathfrak{t}(\omega_\theta)}{1/\mathfrak{c}_0 - \mathfrak{r}(\omega_\theta)} + O(\varepsilon^2),$$

where, recalling Definition 2.5 and (2.9)*,*

$$1/\mathfrak{c}_0 = -\frac{\log(\eta_0\omega_\theta\varepsilon\,\mathrm{cap}\,\partial B)}{2\pi}, \quad \mathfrak{t}(\omega_\theta) = \frac{|U_\theta(z)|^2}{2\omega_\theta}, \quad \mathfrak{r}(\omega_\theta) = \sum_{\substack{j=1\\ j\neq\theta}}^{\infty}\frac{U_j(z)\cdot\mathcal{D}_\Omega^{\omega_\theta}[U_j](z)}{\omega_\theta^2-\omega_j^2};$$

(ii) For ε small enough, we can deduce that $\omega_{\varepsilon,1} \geq \omega_\theta$.

Proposition 2.10. *If ω_θ has double multiplicity then*

$$\omega_{\varepsilon,2} - \omega_\theta = \frac{\mathfrak{t}(\omega_\theta)}{1/\mathfrak{c}_0 - \mathfrak{r}(\omega_\theta)} + O(\varepsilon^2),$$

$$\omega_{\varepsilon,1} - \omega_\theta = O(\varepsilon^2).$$

We notice that by considering an expansion in powers of $1/\log(\varepsilon)$, we obtain

$$\frac{\mathfrak{t}(\omega_\theta)}{1/\mathfrak{c}_0 - \mathfrak{r}(\omega_\theta)} + O(\varepsilon^2) = -\frac{1}{\log\varepsilon}\frac{\pi|U_\theta(z)|^2}{\omega_\theta} + O\left(\frac{1}{\log(\varepsilon)^2}\right).$$

In particular, substituting $2\omega_\theta \simeq \omega_\epsilon + \omega_\theta$ gives back (2.1).

We also notice that if z is on a nodal set of U_θ (i.e. $u_{\theta,1}, \ldots, u_{\theta,m_\theta}$ are all zero at z) then $\mathfrak{t}(\omega_\theta) = 0$, and thus in both the cases of a simple or a double eigenvalue, the splitting order will be $O(\varepsilon^2)$.

Numerical validation for a disk domain and a disk inclusion

Let Ω be the unit disk and let ω_θ^2 be its first non-zero eigenvalue. It is known that ω_θ is given by the first root of the derivative of the Bessel function J_1 and has double multiplicity. Suppose that also the rescaled inclusion B is a unit disk.

In Figure 2.1, we compare results obtained through the multipole expansion method with the ε^2 error given by the formula for $\omega_{\varepsilon,1} - \omega_\theta$. The multipole expansion is implemented by setting two polar coordinate systems, one centered in the center of Ω and one in z, and exploiting Graf's summation formula for Bessel functions to rewrite the eigenvalue problem as a root search for the determinant of the coordinate transformation matrix.

In Figures 2.2 and 2.3, we compare asymptotic formulae for $\omega_{\varepsilon,2} - \omega_\theta$ with results obtained with the multipole expansion method. The asymptotic formula is implemented numerically by truncating at a finite value the series in the definition of $\mathfrak{r}(\omega_\theta)$ in (2.7), and approximating the boundary layer integrals in $\mathfrak{r}(\omega_\theta)$ by quadrature.

We remark that the improved resolution of the inclusion size and position opens the possibility of the development of accurate inclusion reconstruction algorithms using the asymptotic formulae from Propositions 2.9 and 2.10. Of particular interest, also in applications, would be the development of an efficient reconstruction method for locating and characterizing small inclusions based only on the knowledge of eigenvalues shift. The implementation of such a method and its applications are studied in Chapter 5.

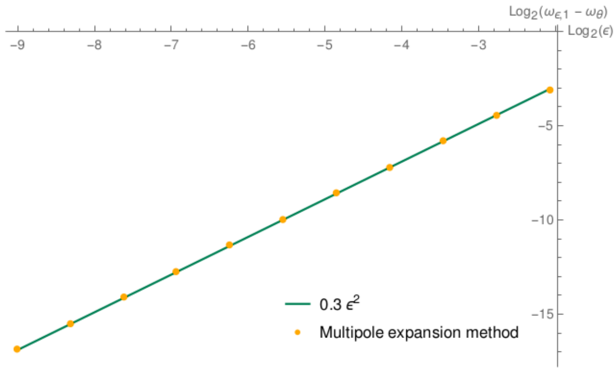


Figure 2.1: A $\log_2$-$\log_2$ plot of $\omega_{\varepsilon,1} - \omega_\theta$ as the size of the inclusion varies and the center is fixed (at $|z| = .5$).

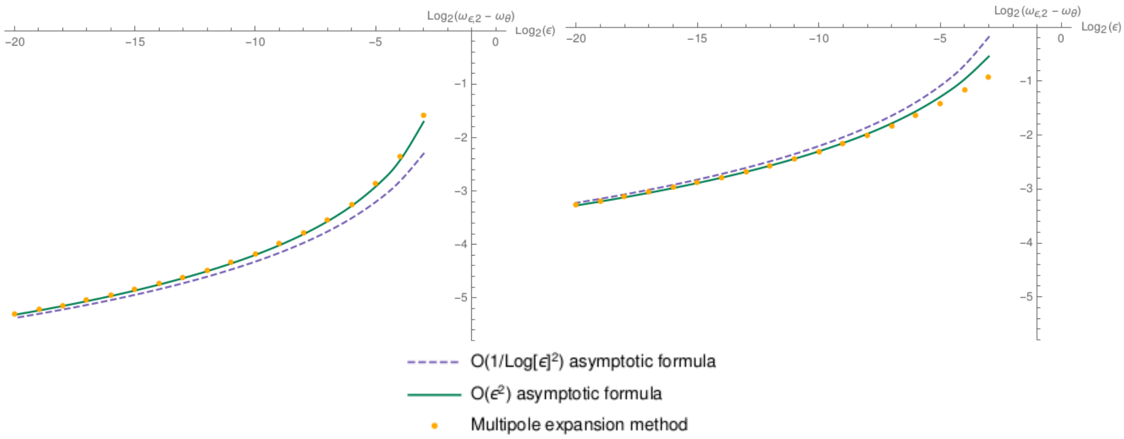


Figure 2.2: A $\log_2$-$\log_2$ plot of the shift $\omega_{\varepsilon,2} - \omega_\theta$ as the size of the inclusion varies and its center remains constant (left at $|z| = .3$, right at $|z| = .8$).

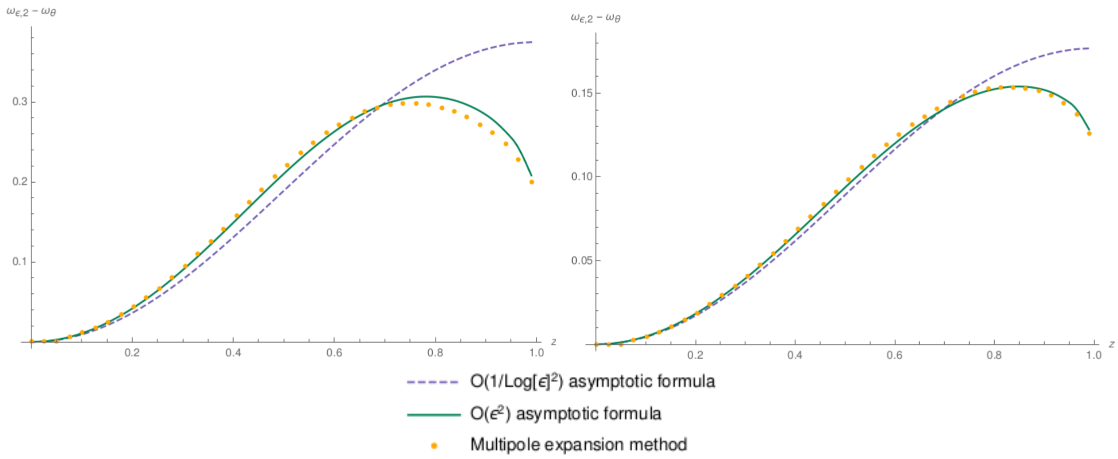


Figure 2.3: A plot of the shift $\omega_{\varepsilon,2} - \omega_\theta$ as the distance from the origin of the center of the inclusion varies and its size remains constant (left at $\varepsilon = 10^{-2}$, right at $\varepsilon = 10^{-4}$).

Chapter 3

Arbitrarily small domain perturbations which split the spectrum of the Laplacian

In the seminal works [79] and [96], respectively Micheletti and Uhlenbeck showed that the eigenvalues of the Dirichlet Laplacian are generically simple in the space of smooth manifolds equipped with the C^k-topology (for subsequent works see also [80], the survey papers [33, Section 4.3], [52, Section 1.3] and references therein). In this chapter, we prove that a localized version of this result holds as follows, even for non-smooth domains.

Theorem 3.1. *For any Lipschitz domain Ω and for any open set U whose intersection with Ω is not empty, there exists a domain $\tilde{\Omega}$ whose symmetric difference with Ω is contained in U and whose Dirichlet/Neumann/Robin Laplacian eigenvalues are all simple. Moreover if $U \cap \partial\Omega$ is not empty, then $\tilde{\Omega}$ can be taken to be bi-Lipschitz homeomorphic to Ω.*

More in detail, the structure of the chapter is the following. In Section 3.1, we review some preliminary material, in particular regarding spectral stability. In Section 3.2, we recall a Hadamard's formula and study independence properties of some expressions involving eigenfunctions and their gradients at the boundary. More specifically, Hadamard's formula provides us with a first-order estimate on the shift of an eigenvalue λ, and which depends on the quantity

$$|\nabla u|^2 - hu^2 \tag{3.1}$$

at the boundary of the domain considered, where u is an eigenfunction associated to λ and h is a function which depends on the choice of boundary conditions. By showing that for two orthogonal eigenfunctions, the corresponding values of (3.1) must differ at least at a point, we are able to construct a localized perturbation which splits any non-simple eigenvalue. However, even when small, this perturbation might cause the shift and the overlap of other eigenvalues. This possibility is ruled out in Section 3.3, where uniform bounds for the whole spectrum are adapted to our case from sharp stability estimates from [32]. These bounds allow the construction of a localized perturbation, which consists in a sequence of successive smaller "bumps" at the boundary of a part cut out from Ω, which proves the first statement of Theorem 3.1. We prove its second statement in Section 3.4, where we use an additional result from [81] which allows us to deform appropriately directly the boundary of $\partial\Omega$, without requiring any topological change of Ω.

We remark that under homogeneous Dirichlet boundary conditions, the splitting of an eigenvalue by the application of Holmgren's uniqueness Theorem and Hadamard's formula is a well-known technique (see for instance [57, Lemma 2.5.9]); also in the case of homogeneous Robin boundary conditions with a never-vanishing impedance coefficient the arguments of [81] can be easily adapted for the same purpose (see the proof of Proposition 3.10). Thus, our efforts will be devoted mainly to the analysis of the novel cases of homogeneous Neumann boundary conditions and of *localized* domain perturbations.

3.1 Preliminaries

We collect here some definitions which will be used extensively in the chapter.

(i) We say that λ is an *eigenvalue* of a domain Ω with associated *eigenfunction* u if

$$\Delta u + \lambda u = 0 \tag{3.2}$$

in Ω, u is not constant zero, and either one of the following homogeneous boundary conditions is satisfied on $\partial\Omega$:

$$\begin{cases} u = 0 & \text{(Dirichlet)}, \\ \alpha u + \dfrac{\partial u}{\partial \nu} = 0 & \text{(Neumann/Robin)}, \end{cases} \tag{3.3}$$

where α is a constant ($\alpha = 0$ for the Neumann condition, $\alpha > 0$ for the Robin condition), and ν indicates the outward unit normal vector.

(ii) We say that $(\phi_t)_{t\in[0,t_0)}$ is a *deformation* if ϕ_t is a diffeomorphism of $\mathbb{R}^N$, ϕ_t is analytic in t, and $|\phi_t - I|_{\mathrm{C}^2(\mathbb{R}^N)} \leq Ct$ for a certain constant C, for every $t \in [0, t_0)$. We say that $(\phi_t)_t$ is *localized* in U if ϕ_t is the identity outside U for all t.

We actually require (3.2) and (3.3) to be satisfied only in a weak sense, that is: λ is an eigenvalue of Ω with associated eigenfunction u, if u is an element of a function space $V(\Omega)$ and

$$Q_\Omega(u, v) = \lambda \int_\Omega uv, \qquad \text{for every } v \in V(\Omega),$$

where, depending on the choice of boundary conditions, we define

Boundary conditions	$Q_\Omega(u, v)$	$V(\Omega)$
Dirichlet	$\int_\Omega \nabla u \cdot \nabla v$	$\mathrm{H}_0^1(\Omega)$
Neumann/Robin	$\int_\Omega \nabla u \cdot \nabla v + \int_{\partial\Omega} \alpha uv$	$\mathrm{H}^1(\Omega)$

(3.4)

where H^1 is the space of square integrable functions with square integrable distributional gradient and H_0^1 its subspace of trace zero functions. However, from elliptic regularity theory, we know that Laplacian eigenfunctions are analytic inside any open domain; thus (3.2) is satisfied also in the classical sense. Moreover, if Σ is a smooth part of $\partial\Omega$, u is also smooth on Σ (see for example [41, Section 6.3] for proofs of these facts).

Recall that from spectral theory, the eigenvalues of Ω have finite multiplicity and can be arranged in a non-decreasing sequence which tends to infinity, and which we will denote as

$$0 \leq \lambda_1 \leq \lambda_2 \leq \dots,$$

where each eigenvalue is repeated as many times as its multiplicity.

For future reference, we record the following uniqueness result.

Theorem 3.2. *Let u be such that $\Delta u + \lambda u = 0$ in Ω. If $u = 0$ and $\partial u/\partial\nu = 0$ on Σ, an open and smooth subset of $\partial\Omega$, then u is identically zero in the whole Ω.*

We briefly outline the classic argument to prove this fact from Holmgren's uniqueness theorem. Let B be an open ball such that $B \cap \partial\Omega \subseteq \Sigma$. Extending u to 0 in

$B \setminus \Omega$, it is easy to check that $-\Delta u = \lambda u$ in the distributional sense in B. By [60, Theorem 5.3.1], u must be zero also in an open set inside Ω. But then $u = 0$ on the whole Ω by analytic continuation.

3.1.1 Stability of eigenvalues of the Laplacian

In this section, we review some results that show that the spectrum of the Laplacian is continuous under domain perturbations, and give some useful quantitative estimates on the eigenvalues' shifts.

We recall a result of analyticity of eigenvalues and eigenfunctions with respect to a perturbation parameter, which is a consequence of the classic Rellich-Nagy Theorem [90, Theorem 1 at p. 33] (see also [33, Section 4.2] and references therein).

Theorem 3.3. *Let $(\phi_t)_t$ be a deformation and let λ be an eigenvalue of Ω of multiplicity m. Then, there exist $\lambda_t^1 \leq \cdots \leq \lambda_t^m$ and functions $u_t^1, \ldots, u_t^m$ such that for $j = 1, \ldots, m$,*

(i) for any t, λ_t^j is an eigenvalue of $\phi_t(\Omega)$ with associated eigenfunction u_t^j;

(ii) for any t, $\int_{\phi_t(\Omega)} u_t^i u_t^j$ is 1 if $i = j$ and is 0 for every $i \neq j$;

(iii) λ_t^j and u_t^j are analytic in t;

(iv) $\lambda_0^j = \lambda$ and u_0^j is an eigenfunction associated to λ.

Moreover, for any $\delta > 0$ small enough, there is a T such that for any $t < T$ the only eigenvalues of $\phi_t(\Omega)$ in $(\lambda - \delta, \lambda + \delta)$ are $\lambda_t^1, \ldots, \lambda_t^m$.

For our purposes, we will also need a finer estimate on the variation of eigenvalues, as expressed in the following lemma.

Lemma 3.4. *Let ϕ be a diffeomorphism of $\mathbb{R}^N$, let λ_n be the n-th eigenvalue of Ω and $\tilde{\lambda}_n$ be the n-th eigenvalue of $\phi(\Omega)$. Then there exists a constant C, which depends only on the Lipschitz constant of $\partial\Omega$, such that*

$$|\tilde{\lambda}_n - \lambda_n| \leq C \max\{\tilde{\lambda}_n, \lambda_n\}(|\phi - I|_{C^1(\mathbb{R}^N)}).$$

The proof of this estimate can be obtained by repeating the same argument from the proof of [32, Lemma 6.1], only substituting appropriately the bilinear form and the function space with the ones defined in (3.4), depending on the boundary conditions considered.

3.2 Hadamard's formula and boundary properties of eigenfunctions

In this section, we study some independence properties of Laplacian eigenfunctions and of their gradients at the boundary. We first recall a Hadamard's formula for the variation of eigenvalues under a deformation. The dot superscript will indicate differentiation in t.

Lemma 3.5. *Let $(\phi_t)_t$ be a deformation. Let λ_t, u_t be an eigenvalue-eigenfunction pair of $\phi_t(\Omega)$, and suppose both are differentiable in t. Then*

$$\dot{\lambda}_0 = \int_{\partial\Omega} \Big(|\nabla u|^2 - \lambda u^2 + (\partial u/\nu_0)(Hu - 2\partial u/\nu_0)\Big)\nu_0 \cdot \dot{e}_0, \tag{3.5}$$

where $\lambda = \lambda_0$, $u = u_0$, ν_t indicates the outward unit normal vector, e_t the identity on $\phi_t(\partial\Omega)$, and H the mean curvature of $\partial\Omega$.

Hereafter, we briefly prove this fact in the case of Dirichlet or Neumann boundary conditions. The case of Robin conditions requires a finer analysis of the dependence on t of the surfaces $\phi_t(\partial\Omega)$, for which we refer to [51, Identity (9)] or [28, Identities (69) and (57)].

Proof. Let $\Omega_t = \phi_t(\Omega)$ for every t. By the divergence theorem, the distributional gradient of the measure $\mathbb{1}_{\Omega_t}\mathcal{L}^N$ is given by $\nu_t\Sigma_t^{N-1}$, where $\mathbb{1}_{\Omega_t}$ is the characteristic function of Ω_t, $\mathcal{L}^N$ is the N-dimensional Lebesgue measure, and Σ_t^{N-1} is the surface measure on $\partial\Omega_t$. Therefore, by the chain rule,

$$\frac{d}{dt}(\mathbb{1}_{\Omega_t}\,\mathcal{L}^N) = \nu_t \cdot \dot{e}_t\,\Sigma_t^{N-1},$$

so we have the following Leibniz' formula:

$$\frac{d}{dt}\left(\int_{\Omega_t} f_t\right) = \int_{\Omega_t} \dot{f}_t + \int_{\partial\Omega_t} f_t\nu_t \cdot \dot{e}_t. \tag{3.6}$$

Consider now the identity

$$\lambda_t = -\int_{\Omega_t} u_t\Delta u_t = \int_{\Omega_t} |\nabla u_t|^2. \tag{3.7}$$

Differentiating in t the first equality in (3.7) and using (3.6), we obtain

$$2\lambda_t \int_{\Omega_t} \dot{u}_t u_t = -\lambda_t \int_{\partial\Omega_t} u_t^2\nu_t \cdot \dot{e}_t. \tag{3.8}$$

In the case of Neumann boundary conditions, differentiating in t the last term in (3.7), using (3.6), integrating by parts, and substituting (3.8), we have that

$$\dot{\lambda}_t = \int_{\partial\Omega_t} (|\nabla u_t|^2 - \lambda_t u_t^2)\nu_t \cdot \dot{e}_t + 2\int_{\partial\Omega_t} \dot{u}_t \frac{\partial u_t}{\partial \nu_t},$$

which gives (3.5) since $\partial u_0/\partial\nu_0 = 0$ on $\partial\Omega_0$. Proceeding in the same way for Dirichlet boundary conditions, only exchanging the roles of the functions in the integration by parts step, we obtain

$$\dot{\lambda}_t = \int_{\partial\Omega_t} (|\nabla u_t|^2 - \lambda_t u_t^2)\nu_t \cdot \dot{e}_t + 2\int_{\partial\Omega_t} u_t \frac{\partial \dot{u}_t}{\partial \nu_t} + 2\dot{\lambda}_t,$$

which gives (3.5), since $u_0 = 0$ on $\partial\Omega_0$. □

We notice that considering

$$h = \begin{cases} 0 & \text{if } u = 0 \text{ on } \partial\Omega, \\ \lambda + \alpha H + 2\alpha^2 & \text{if } \alpha u + \partial u/\nu = 0 \text{ on } \partial\Omega, \end{cases} \tag{3.9}$$

the integrand in parentheses in (3.5) can be rewritten as $|\nabla u|^2 - hu^2$. In the following lemma we study such a quantity, in particular the behavior of its zeros.

Lemma 3.6. *Let E be a smooth domain and let S be a connected component of its boundary. Let u and v be two orthonormal eigenfunctions of E, associated to the same eigenvalue λ. Let H be the mean curvature of S and let h be as in* (3.9)*. Then, under Dirichlet or Neumann boundary conditions, neither of the quantities*

$$|\nabla u|^2 - hu^2, \tag{3.10}$$

$$|\nabla u|^2 - hu^2 - (|\nabla v|^2 - hv^2), \tag{3.11}$$

can be identically zero on S. The same statement holds in the case of Robin boundary conditions under the additional requirement that the mean curvature satisfies $-\alpha H < \alpha^2 + \lambda$.

Proof. Suppose that (3.10) is zero on S. If the Dirichlet condition holds, then $\partial u/\partial\nu = u = 0$ on S. Thus, by Theorem 3.2 we have that $u = 0$ in E, which is a contradiction.

If the Neumann condition holds, then from the assumption that (3.10) is zero, we have

$$|\nabla_S u|^2 = \lambda u^2, \tag{3.12}$$

where ∇_S is the surface gradient on S. By Theorem 3.2, the eigenfunction u cannot be constant zero on S, so there exists a point $x_0 \in S$ such that $u(x_0) \neq 0$. The approach we follow hereafter is inspired by [58, Chapter 6]. Let $\gamma : (-\infty, +\infty) \to S$ be a solution of the Cauchy problem

$$\begin{cases} \gamma_0 = x_0, \\ \dot{\gamma}_t = (\nabla_S u)(\gamma_t). \end{cases}$$

Existence and uniqueness of such a γ for every t is guaranteed by standard results in the theory of ordinary differential equations on surfaces, since by assumption S is a compact, maximally connected, smooth hypersurface and ∇u is smooth on S. Then, by the chain rule and (3.12), we have the differential equation

$$\frac{du(\gamma_t)}{dt} = |\nabla_S u|^2(\gamma_t) = \lambda u(\gamma_t)^2, \tag{3.13}$$

which is solved, once imposed the initial condition $u_0 = u(\gamma_0)$, by

$$u(\gamma_t) = \frac{1}{1/u_0 - \lambda t}.$$

But this would lead to the blow up of u for $t \to 1/(\lambda u_0)$, which contradicts the boundedness of u on S.

If the Robin condition holds, with the same reasoning we can obtain (3.13) only with λ substituted by $h - \alpha^2$. By the assumption on the mean curvature, we have that $h - \alpha^2 > 0$, and therefore $du(\gamma_t)/dt \geq cu(\gamma_t)^2$ for some positive constant c. Thus u would need to blow up in finite time, which is impossible.

The proof that (3.11) is not constant zero on S employs similar considerations. Suppose that (3.11) is zero on S. In the case the Dirichlet condition holds, this implies that $(\partial u/\nu)^2 = (\partial v/\nu_0)^2$. Then Theorem 3.2 implies that $u = \pm v$ in E. This contradicts the orthogonality assumption of u and v.

In the case the Neumann condition holds, the assumption that (3.11) is zero implies that

$$|\nabla_S u|^2 - |\nabla_S v|^2 = \lambda(u^2 - v^2) \text{ on } S. \tag{3.14}$$

By Theorem 3.2 and continuity of u, v, there exists a point $x_0 \in S$ such that $u(x_0)$ and $v(x_0)$ are different and non-zero. By eventually switching them or changing the sign of u, v, we can suppose that $u(x_0) > v(x_0) > 0$. Let $k = u(x_0) + v(x_0) > 0$ and let $\gamma : (-\infty, \infty) \to S$ be a solution of

$$\begin{cases} \gamma_0 = x_0, \\ \dot{\gamma}_t = (\nabla_S u + \nabla_S v)(\gamma_t). \end{cases}$$

Let $f_t = u(\gamma_t), g_t = v(\gamma_t)$. Then, by the chain rule, it holds

$$\frac{d(f_t + g_t)}{dt} = |\nabla_S u + \nabla_S v|^2(\gamma_t) \geq 0, \tag{3.15}$$

so $f_t + g_t > k$ for every $t > 0$. Then

$$\frac{d(f_t - g_t)}{dt} = (|\nabla_S u|^2 - |\nabla_S v|^2)(\gamma_t) = \lambda(f_t - g_t)(f_t + g_t) \geq \lambda k(f_t - g_t), \tag{3.16}$$

which, since $f_0 - g_0 > 0$, would lead to $f_t - g_t \to \infty$ as $t \to \infty$, which contradicts the boundedness of u and v.

If the Robin condition holds, then by reasoning as before, we obtain the same chain of equalities as in (3.16) only with λ substituted by $h - \alpha^2$, that is

$$\frac{d(f_t - g_t)}{dt} = (h - \alpha^2)(f_t - g_t)(f_t + g_t).$$

Since $f_t + g_t > k \geq 0$ for $t > 0$ by (3.15), and the mean curvature bound assumption $-\alpha H < \alpha^2 + \lambda$ implies that $h - \alpha^2 > 0$, then there exists a positive constant c such that

$$\frac{d(f_t - g_t)}{dt} \geq c(f_t - g_t),$$

which, since $f_0 - g_0 > 0$, would lead again to the unboundedness of $f_t - g_t = u(\gamma_t) - v(\gamma_t)$ as $t \to \infty$, which is impossible. $\square$

3.3 Splitting by a perturbation of the boundary of a hole

In this section, we cut a circular hole inside Ω and deform its boundary to split the spectrum of the perturbed domain. We start by constructing a deformation of Ω minus a part which splits a single eigenvalue as follows.

Proposition 3.7. *Let G be a smooth domain whose closure is contained in Ω. Let λ be an eigenvalue of $\Omega \setminus \overline{G}$ of multiplicity m. In the case of Robin conditions suppose that H, the mean curvature of ∂G, satisfies $\alpha H < \alpha^2 + \lambda$. Then for any open set U containing $\overline{G}$, and any choice of different indices i, j among $1, \ldots, m$, there exists a deformation $(\phi_t)_t$ localized in U such that (with the notation of Theorem 3.3 with Ω replaced by $\Omega \setminus \overline{G}$) the eigenvalues $\lambda_t^1, \ldots, \lambda_t^m$ of $\phi_t(\Omega \setminus \overline{G})$ are such that $\lambda_t^i \neq \lambda_t^j$ for all $t \in (0, t_0)$.*

Proof. Let h be as in (3.9) and let $S = \partial G$. Let $u_t^1, \dots, u_t^m$ be the eigenfunctions associated to the eigenvalues $\lambda_t^1, \dots, \lambda_t^m$ as in Theorem 3.3. By Lemma 3.6, there exists y on S such that

$$(|\nabla u_0^i|^2 - h(u_0^i)^2)(y) \neq (|\nabla u_0^j|^2 - h(u_0^j)^2)(y). \tag{3.17}$$

Then, by choosing a deformation $(\phi_t)_t$ which is the identity outside an appropriately small neighborhood of y, we have

$$\int_S (|\nabla u_0^i|^2 - h(u_0^i)^2)\, \nu \cdot \dot{\phi}_0 \neq \int_S (|\nabla u_0^j|^2 - h(u_0^j)^2)\, \nu \cdot \dot{\phi}_0. \tag{3.18}$$

Such a deformation can be constructed in many ways (for the sake of completeness, we give an explicit example hereafter). By Lemma 3.5, (3.18) implies that $\dot{\lambda}_0^i \neq \dot{\lambda}_0^j$. Since λ_t^i and λ_t^j are both analytic in t, we conclude that there exists t_0 such that $\lambda_t^i \neq \lambda_t^j$ for $t \in (0, t_0)$.

We show how to build a deformation such that (3.18) holds. Let ψ be a diffeomorphism so that

$$\psi(B_1 \cap \{x_N < 0\}) = V \cap \Omega,$$

where B_1 is the unit ball and V a small neighborhood of y. Let $\hat{z}$ indicate $(z_1, \dots, z_{N-1})$ and let

$$\rho_c(\hat{z}) = \begin{cases} \dfrac{c^3}{8} \exp\left(\dfrac{1}{|\hat{z}/c|^2 - 1}\right) & \text{if } |\hat{z}| < c, \\ \\ 0 & \text{otherwise.} \end{cases}$$

Notice that by construction $|\rho_c|_{\mathrm{C}^2(\mathbb{R}^{N-1})} \leq c$ for any $c \leq 1$. Let $\varphi_t(z)$ be the extension of the map $z \mapsto (\hat{z}, t\rho_c(\hat{z}))$ from $\{x_N = 0\}$ to a diffeomorphism which is the identity outside B_1 and such that $|\varphi_t - I|_{\mathrm{C}^2(\mathbb{R}^N)} \leq ct$. Let $\phi_t = \psi \circ \varphi_t \circ \psi^{-1}$. Then by taking $c \leq |\psi|_{\mathrm{C}^2} |\psi^{-1}|_{\mathrm{C}^2}$, we have

$$|\phi_t - I|_{\mathrm{C}^2} \leq t. \tag{3.19}$$

By eventually considering a smaller c, the continuity of u on S together with (3.17) imply that (3.18) holds. $\square$

Although Proposition 3.7 shows how to split an eigenvalue, the perturbation chosen might cause two other eigenvalues to overlap, creating a new repeated one. To avoid this potential issue, we need a finer control on the behavior of the whole spectrum. This is what is achieved in the following lemma.

Lemma 3.8. *Let G be a smooth domain whose closure is contained in Ω. We indicate as $\lambda_1 \le \lambda_2 \le \dots$ the eigenvalues of $\Omega \setminus \overline{G}$, and as r the first index such that λ_r has multiplicity $m \ge 2$. In the case of Robin conditions, suppose that H, the mean curvature of G, satisfies $\alpha H < \alpha^2 + \lambda$. Then, for any open set U which contains G and any $\varepsilon > 0$, there exists $(\phi_t)_t$ a deformation localized in U such that, indicating as $\lambda_1^t \le \lambda_2^t \le \dots$ the eigenvalues of $\phi_t(\Omega \setminus \overline{G})$, for all $t \le t_0$ we have that*

(i) for all $i \le r + m + 1$ it holds

$$|\lambda_i^t - \lambda_i| \le \varepsilon d_r,$$

where d_r is the minimum positive number of $\{\lambda_{j+1} - \lambda_j : j = 1, \dots, r+m\}$;

(ii) the multiplicity of λ_r^t is strictly smaller than the multiplicity of λ_r;

(iii) for all $i > r + m$, it holds $\lambda_i^t > \lambda_r$.

Proof. Let $(\phi_t)_t$ be a deformation as given by Proposition 3.7. Let $u_1^t, u_2^t, \dots$ be the eigenfunctions of $\Omega \setminus \overline{G}$ associated respectively to $\lambda_1^t, \lambda_2^t, \dots$. By Theorem 3.3, we can assume that λ_i^t, u_i^t are analytic in t, that $\lambda_i^0 = \lambda_i$, and that $u_r^0, \dots, u_{r+m}^0$ is an orthonormal basis for the eigenspace of λ_r. Then, there are two distinct indices i and j among $\{r, \dots, r+m\}$, such that for t_0 small enough,

$$\lambda_i^t \ne \lambda_j^t, \qquad \text{for } t \in (0, t_0]. \tag{3.20}$$

By the eigenvalue stability estimate of Lemma 3.4, there is a t_0 small enough such that

$$|\lambda_i^t - \lambda_i| \le \varepsilon d_r, \quad \forall t \le t_0, \forall i \in \{1, \dots, r+m+1\}. \tag{3.21}$$

Let C, C' indicate two constants which depend only on the dimension N, the Lipschitz constant of $\partial(\Omega \setminus \overline{G})$ and the area of Ω. By Weyl's asymptotic law, $\lambda_n = Cn^{2/N} + o(n^{2/N})$ for any n. Then, from the uniform estimate of Lemma 3.4, it follows that, for $i > r + m$,

$$\lambda_i^t - \lambda_r \ge (\lambda_i^t - \lambda_i) + \lambda_i - \lambda_r \ge C'(-Cci^{2/N} + i^{2/N} - r^{2/N}),$$

where $c > 0$ is a bound on the deformation magnitude which we can make arbitrarily small by taking a smaller t_0. Therefore, for t_0 and c small enough,

$$\lambda_i^t - \lambda_r > 0, \quad \forall t \le t_0, \forall i > r + m. \tag{3.22}$$

In conclusion, Items i-ii-iii are consequences of (3.21)-(3.20)-(3.22). $\square$

The construction in the previous proof gives us a method to split the first non-simple eigenvalue without altering the simplicity of smaller eigenvalues. In fact, by taking $\varepsilon < 1/2$, from Items i and iii of Lemma 3.8, we have that the eigenvalues λ_i^t perturbed from λ_i:

- lie in disjoint neighborhoods of λ_i, for $i < r$;
- are not further than $d_r/2$ from λ_i, for $r \leq i \leq r+m$;
- are larger than λ_r, for $i > r+m$.

We can iterate this procedure to split the whole spectrum as in the following proof. Some additional care must be taken in the case of Robin boundary conditions.

Proof of the first statement of Theorem 3.1. Let G_0 be a ball of radius R contained in U. We consider the following recursive construction: let $G_n = \phi^n_{t_n}(G_{n-1})$ where the deformation ϕ^n_t is the one obtained by Lemma 3.8 with G, ε substituted respectively by G_{n-1}, ε_n. By choosing ε_n small enough at each step, we have that $\partial G_n \to \partial E$ in C^2-norm, where E is a smooth domain contained in U. In the case of Robin boundary conditions, notice that the mean curvature H_0 of G_0 is $-(N-1)/R$ and satisfies $\alpha H_0 < \alpha^2 + \lambda$ for any eigenvalue $\lambda > 0$, since we assumed $\alpha \geq 0$. Moreover, by eventually choosing a smaller ε_n for each n, thanks to (3.19) we can assume the mean curvature of G_n is still negative, so that the assumptions of Lemma 3.8 hold at every step for any boundary condition. Let $\tilde{\Omega} = \Omega \setminus \overline{E}$.

Let r_n be the index of the first non-simple eigenvalue of $\Omega \setminus \overline{G}_n$. By Items i and iii of Lemma 3.8 we have that all eigenvalues with index smaller than r_n are simple for every n. Moreover, $(r_n)_n$ is a non-decreasing sequence of integers which can not be definitely constant; in fact by Item ii of Lemma 3.8, r_{n+j} can be equal to r_n for at most $j \in \{1, \dots, r_n\}$. Therefore, $r_n \to \infty$ as $n \to \infty$, and thus $\tilde{\Omega}$ can have only simple eigenvalues. $\square$

We remark that our previous construction involves cutting out a part of Ω which causes $\tilde{\Omega}$ to be not homeomorphic to Ω. However, this can be avoided by deforming appropriately the boundary of Ω, instead of the boundary of the hole, as shown in the following section.

3.4 Splitting by a perturbation of the boundary

In this section, we show how to deform directly a part of the boundary of Ω to split its spectrum.

Let U be an arbitrary open set whose intersection with $\partial\Omega$ is non-empty. By eventually applying a bi-Lipschitz transformation which modifies Ω only in U, we can assume, and will do so, that there is an open set $V \subseteq U$ such that $\Sigma = V \cap \partial\Omega$ is contained in a hyperplane.

We recall now a result proved in [81, Lemma 6 and calculations leading to (20)], which relies on the explicit computation of the Fréchet derivative of the bilinear form $Q_{\psi(\Omega)}$ with respect to ψ and on properties of Fredholm operators.

Lemma 3.9. *Let $(\phi_t)_t$ be a deformation localized in V. Under the same notation of Theorem 3.3, if for every $t \leq t_0$ we have that $\lambda_t^1 = \cdots = \lambda_t^m$, then the matrix with element*

$$\int_\Sigma (\nabla u_0^k \cdot \nabla u_0^l)\phi_t \cdot \nu - \alpha f u_0^k u_0^l \, \nu \cdot \nabla\phi_t \nu \tag{3.23}$$

in position (k, l), where f is a positive continuous function, is a multiple of the identity matrix for every $t \leq t_0$.

With the aid of the previous lemma, we can construct a deformation which splits a single eigenvalue as follows.

Proposition 3.10. *Let λ be an eigenvalue of Ω of multiplicity $m \geq 2$. Then, with the notation of Theorem 3.3, there are two indices i, j and there exists a deformation $(\phi_t)_t$ localized in V such that $\lambda_\varepsilon^i \neq \lambda_\varepsilon^j$ for a certain $\varepsilon < t_0$.*

Proof. In the case of Dirichlet conditions, the construction is the same as the one considered in Section 3.3, only with the deformation applied directly to the boundary of $\partial\Omega$. In fact, in this case the existence of a point $y \in \Sigma$ such that (3.17) holds is guaranteed directly by Theorem 3.2. Then the claim in the conclusion can be obtained by constructing a deformation in a small neighborhood of y exactly as in Proposition 3.7.

In the case of Neumann conditions, if there exists a point $y \in \Sigma$ such that (3.17) holds, we can again build a local deformation of the boundary which fulfils our thesis. If instead

$$|\nabla u_0^k|^2 - \lambda(u_0^k)^2 = |\nabla u_0^l|^2 - \lambda(u_0^l)^2 \tag{3.24}$$

on Σ for every k, l, we show that we can find anyway indices i, j and a deformation $(\phi_t)_t$ such that $\lambda_\varepsilon^i \neq \lambda_\varepsilon^j$ for some ε. In fact, if we suppose by contradiction that this is not the case, then by taking $\nu \cdot \nabla\phi_t\nu = 0$ and by the arbitrariness of $\phi_t \cdot \nu$ in (3.23), Lemma 3.9 would lead to $|\nabla u_k|^2 = |\nabla u_l|^2$ on Σ for every k, l. If $\lambda = 0$ then it has already multiplicity 1. If $\lambda \neq 0$ then (3.24) would become $(u_0^k)^2 = (u_0^l)^2$ on Σ, which by Theorem 3.2 would lead to $u_0^k = \pm u_0^l$ in Ω, which is a contradiction.

The case of Robin boundary conditions can be proven from Lemma 3.9 alone. If there was no deformation $(\phi_t)_t$ localized in V which splits the eigenvalue λ, by choosing $\phi_t \cdot \nu = 0$ and $\nu \cdot \nabla\phi_t\nu$ arbitrarily, making use of Lemma 3.9 we would have

$$u_0^k u_0^l = 0 \text{ for } k \neq l, \qquad (u_0^k)^2 = (u_0^l)^2 \text{ for every } k, l,$$

which would lead to $u_0^k = -\alpha(\partial u_0^k/\partial\nu) = 0$ on Σ, which is prohibited by Theorem 3.2. □

Finally we can easily adapt the arguments from Section 3.3 to construct a localized boundary perturbation which splits the spectrum.

Proof of the second statement of Theorem 3.1. Let $(B_n)_n$ be a sequence of mutually disjoint balls contained in V such that $B_n \cap \partial\Omega$ is non-empty for every n. By Proposition 3.10 and by the same reasoning as in the proof of Lemma 3.8, we can build a deformation ϕ_t^1 localized in B_1 such that for a certain $t = t_1$, Items i-ii-iii of Lemma 3.8 hold. Letting $\Omega_1 = \phi_{t_1}^1(\Omega)$, we can repeat again the same construction to build a deformation ϕ_t^2 localized in B_2 and obtain a new domain $\Omega_2 = \phi_{t_2}^2(\Omega_1)$. Iterating this construction, we obtain a sequence of domains Ω_n which coincide with Ω outside V and whose boundaries converge in C^1-norm inside V. The limit domain is thus bi-Lipschitz equivalent to Ω and, by the same concluding argument of the proof of the first statement of Theorem 3.1, has a simple spectrum. □

Chapter 4

Extending asymptotic formulae from simple to repeated eigenvalues

Many asymptotic formulae for the shift of eigenvalues of elliptic differential operators caused by small singular perturbations have been obtained in the case of multiplicity one (see for instance [77, Chapter 9], [14] and references therein, [86], [87], [47]). The generalization of such expressions to higher multiplicities often requires non-trivial calculations and is restricted to specific cases (see for example [76], [22], [57, Theorem 2.5.8]). Moreover, such an effort is usually considered unnecessary due to genericity results of simple eigenvalues (see [79], [80], [96], [95]). Nonetheless, higher multiplicities appear in many natural situations; for instance the Laplacian has non-simple spectrum whenever the domain presents some symmetries. In this chapter, we derive a new tool to study the behaviour and properties of repeated eigenvalues for general types of perturbations. Namely, the main result is a variational characterization (Theorem 4.7) which allows the direct extension of asymptotic formulae which are valid for simple eigenvalues to non-simple ones. We then apply this result to study different domain perturbations of interest in applications.

The chapter is organized as follows. In Section 4.1.1, we recall some results regarding the spectral stability and generic simplicity for second-order elliptic operators. In Section 4.2, we derive the main variational characterization by a technique which involves a double perturbation at asymptotically different speeds. Finally in Section 4.3, we consider some domain perturbations of particular interest in applications: grounded inclusions, conductivity inclusions, and boundary deformations. We show how the general variational asymptotic formula applies in each of these cases and derive new interesting properties for the Dirichlet and Neumann Laplacian eigenvalues. We refer to Section 4.3.4 for a more specific summary of the results obtained for these two cases.

4.1 Preliminaries

We briefly recall three types of convergence of domains. We say that Ω_ε converges to Ω as $\varepsilon \to 0$ in:

- Hausdorff distance, if $d_H(\Omega_\varepsilon, \Omega) \to 0$, where

$$d_H(A, B) = \max\{\sup_{a\in A}\inf_{b\in B} |a-b|,\ \sup_{b\in B}\inf_{a\in A} |a-b|\};$$

- measure, if $|\Omega_\varepsilon \vartriangle \Omega| \to 0$, where $\vartriangle$ indicates symmetric difference and $|\cdot|$ the Lebesgue measure;

- C^k-topology, if there is a family $(\phi_\varepsilon)_\varepsilon$ of functions in $\mathrm{C}^k(\mathbb{R}^d, \mathbb{R}^d)$ such that

$$\Omega + \phi_\varepsilon(\Omega) = \Omega_\varepsilon \quad \text{and} \quad |\phi_\varepsilon|_{\mathrm{C}^k} \xrightarrow{\varepsilon\to 0} 0. \tag{4.1}$$

We collect hereafter some relationships between these types of convergence which are relevant to us. C^k-convergence implies Hausdorff convergence, since if (4.1) holds then $d_H(\Omega_\varepsilon, \Omega) \leq |\phi_\varepsilon(\Omega)|_{\mathrm{C}^0} \xrightarrow{\varepsilon\to 0} 0$. If the sets considered have Lipschitz and connected boundaries, Hausdorff convergence implies measure convergence, since in this case $|\Omega_\varepsilon \vartriangle \Omega| \leq d_H(\Omega_\varepsilon, \Omega) \min\{|\Omega_\varepsilon|, |\Omega|\}$. Although the converse result fails in general, if the converging sequence's boundaries have uniformly bounded Lipschitz constants, then, by a local patching argument, it can be easily shown that also measure convergence implies Hausdorff convergence. Therefore, although we will state all our results referring to Hausdorff convergence, they can be adapted to other types of convergence whenever the domains under consideration have enough regularity.

4.1.1 Stability and simplicity of the spectrum of second-order elliptic operators

Let $L(\Omega)$ be a second-order, self-adjoint, elliptic differential operator defined on Ω and let a be its associated coercive, continuous, and bounded bilinear form. We say that λ is an eigenvalue of $L(\Omega)$ with associated eigenfunction $u \in V(\Omega)$ if

$$a(u,v) = \lambda \int_\Omega uv, \qquad \forall v \in V,$$

where $V(\Omega) = \mathrm{H}^1_0(\Omega)$ in the case of homogeneous Dirichlet boundary conditions, or $V(\Omega) = \mathrm{H}^1(\Omega)/\mathbb{R}$ in the case of homogeneous Neumann boundary conditions. From standard results in spectral theory, we know that the eigenvalues of an elliptic operator defined on a Lipschitz domain have finite multiplicity and can be arranged in a non-decreasing sequence. We also assume that the associated eigenfunctions are orthonormal in $\mathrm{L}^2(\Omega)$. With these conventions, we can state the following stability result.

Theorem 4.1. *For every $\varepsilon > 0$, let L be an elliptic operator and let ρ_ε be a smooth function with support contained in Ω such that its C^2-norm is smaller than ε. For any $n \in \mathbb{N}$, let λ be the n-th eigenvalue of L and λ_ε be the n-th eigenvalue of $L + \rho_\varepsilon$, and let u_ε be an associated eigenfunction. Then there exists a constant C such that for every ε small enough*

$$|\lambda_\varepsilon - \lambda| \leq C\varepsilon,$$

and there exists u, an eigenfunction of λ, such that

$$|u_\varepsilon - u|_{\mathrm{H}^1(\Omega)} \leq C\varepsilon.$$

The proof is a consequence of standard results in perturbation theory (see for instance [90, Theorem 1 at p.57]). We are interested not only in stability with respect to smooth perturbations of coefficients but also in singular perturbations of domains. In particular, we will need the following result.

Theorem 4.2. *Let Ω and Ω_ε be two Lipschitz domains whose Hausdorff distance one from another is ε. Let $L(\Omega)$ and $L(\Omega_\varepsilon)$ be second-order elliptic operators with homogeneous Dirichlet or Neumann boundary conditions imposed on $\partial\Omega$ and $\partial\Omega_\varepsilon$. Let M be an upper bound to the Lipschitz constants of $\partial\Omega$ and $\partial\Omega_\varepsilon$, and to the coercivity, continuity and boundedness constants of a. For any $n \in \mathbb{N}$, let λ be the*

n-th eigenvalue of $L(\Omega)$ and λ_ε be the n-th eigenvalue of $L(\Omega_\varepsilon)$. Then there exists a constant C which depends only on M, n, and the dimension d such that

$$|\lambda_\varepsilon - \lambda| \leq C\varepsilon. \tag{4.2}$$

A proof of this result can be obtained as a consequence of the theory of transition operators and its applications (see [33] for a survey of this technique). In what follows, we outline another approach which relies on stability results for boundary value problems.

Outline of the proof. We adapt the argument in [69, Section 4.4] to our case. Let E be an arbitrary Lipschitz domain containing $\Omega_\varepsilon \cup \Omega$ and consider u_ε extended to the whole E. Let u be the orthogonal projection of u_ε from $V(E)$ onto $V(\Omega)$. Let $\overline{u}$ be the unique solution in $V(\Omega)$ of

$$a(\overline{u}, v) = \lambda \int uv, \qquad \forall v \in V(\Omega).$$

From [93, Inequality (3.2)], we have that

$$|\overline{u} - u|_{\mathrm{H}^1(E)} \leq C|\lambda u|_{\mathrm{L}^2(E)}|\lambda u|_{V(E)'} d_H(\Omega, \Omega_\varepsilon),$$

where C is a constant which depends only on the Lipschitz constant of Ω, and the constants involved in the continuity, boundedness and coercivity assumptions on a. Since $|u|_{V(E)'} \leq |u|_{\mathrm{L}^2(E)}$, and by Weyl's law, there is a constant $\tilde{C}$ which depends only on the area of Ω and the dimension d such that $\lambda \leq \tilde{C}n^{d/2}$. Then, it follows that

$$|\overline{u} - u|_{\mathrm{H}^1(E)} \leq C\tilde{C}n^{2/d}|u|^2_{\mathrm{L}^2(E)} d_H(\Omega, \Omega_\varepsilon).$$

Hence, by (4.31) and Lemma 14 of [69], we obtain estimate (4.2). □

The following result concerning stability of eigenfunctions is a particular case of [43, Theorem 1.2 and subsequent discussion].

Theorem 4.3. *Let Ω_ε be a family of Lipschitz domains converging to Ω in Hausdorff distance as $\varepsilon \to 0$. Suppose that at least one of the following hypotheses holds:*

- $\Omega_\varepsilon \subseteq \Omega$ *for every* ε*;*
- *the Lipschitz constants of $\partial\Omega_\varepsilon$ are uniformly bounded.*

Let λ and λ_ε be as in the hypothesis of Theorem 4.2 and let $u_{\varepsilon,1},\dots,u_{\varepsilon,m}$ be an orthonormal basis of the eigenspace of λ_ε. Then there exists $u_1,\dots,u_m$ an orthonormal basis of λ such that as $\varepsilon\to 0$ it holds

$$u_{\varepsilon,j}\to u_j \text{ in } \mathrm{H}^1(\Omega), \qquad \forall j\in\{1,\dots,m\}\,.$$

We move on to the issue of genericity of simple eigenvalues.

Theorem 4.4. *For every $\varepsilon>0$ and every open set $U\subseteq\Omega$ there exists a smooth function ρ with support contained in U such that its C^2-norm is smaller than ε and $L+\rho$ has simple spectrum.*

This result is an immediate consequence of [96, Theorem 7]. We remark that in Chapter 3 we proved genericity of simple eigenvalues by domain deformation, instead of coefficient perturbations. The results which follow could indeed be proved using only domain deformations, but the arguments would require some more attention due to the variation of the underlying domain.

4.2 Variational asymptotic formula

Recall that the eigenvalues and eigenfunctions of L can be characterized respectively as minima and minimizers of a quadratic functional F. More explicitly, if we indicate as $\lambda_1\le\lambda_2\le\dots$ the eigenvalues of L and $u_1,u_2,\dots$ some associated orthonormal eigenfunctions, we have that for $Fu=\langle Lu,u\rangle_V$ it holds

$$u_n\in\operatorname*{argmin}_{u\in U_n} Fu, \qquad \lambda_n = Fu_n, \tag{4.3}$$

where $U_n=\Big\{u\in V\,:\,u\perp\{u_1,\dots,u_{n-1}\}\,,\ |u|_V=1\Big\}$. However, there is an ambiguity in the choice of eigenfunctions which is particularly relevant to us: if $\lambda_n=\dots=\lambda_{n+m}$, any choice of orthonormal eigenfunctions in the linear space spanned by $\{u_n,\dots,u_{n+m}\}$ is still a basis of the eigenspace. Our variational characterization will select the right basis for the problem considered up to a predetermined asymptotic error. More precisely, we make the following assumptions.

Assumption 4.5. We suppose that there is a family of self-adjoint, elliptic, second-order differential operators L_ε which converges spectrally to L as $\varepsilon\to 0$, that is the n-th eigenvalue of L_ε and any of its associated eigenfunctions converge respectively to the n-th eigenvalue of L and to a function in its eigenspace. Moreover, we suppose that there exists an open set on which the differential operators L and L_ε coincide for every ε.

Assumption 4.6. We suppose that we already know an asymptotic expansion for simple eigenvalues. In particular, we assume that if λ is a simple eigenvalue of L with associated eigenfunction u, and if λ_ε is an eigenvalue of L_ε which converges to λ as $\varepsilon \to 0$, then

$$\lambda_\varepsilon - \lambda = f(\varepsilon, u) + r(\varepsilon),$$

where f is a known function and by $r(\varepsilon)$ we indicate a function which is of order $o(f(\varepsilon, u))$ as $\varepsilon \to 0$. We also require f to be continuous.

Under these assumptions, we can derive the following result.

Theorem 4.7 (Variational characterization)**.** *Let λ be an eigenvalue of L of multiplicity m, and let $\lambda_{\varepsilon,1} \leq \cdots \leq \lambda_{\varepsilon,m}$ be the eigenvalues of L_ε which converge to λ as $\varepsilon \to 0$. Then, for any $j \in \{1, \ldots, m\}$, it holds*

$$\lambda_{\varepsilon,j} - \lambda = f(\varepsilon, v_j) + r(\varepsilon),$$

where

$$v_j \in \operatorname*{argmin}_{v \in U_{\lambda,j}} f(\varepsilon, v), \qquad U_{\lambda,j} = \Big\{ v \in V : Lv = \lambda v,\ v \perp \{v_1, \ldots, v_{j-1}\}\,,\ |v|_V = 1 \Big\}. \tag{4.4}$$

Proof. Step 1. By Assumption 4.5, there exists an open ball $B \subseteq \mathbb{R}^d$ on which $L \equiv L_\varepsilon$. For every $\delta > 0$, by Theorem 4.4 there exists $\rho_\delta \in C_c^\infty(B)$ such that $|\rho_\delta|_{C^2} < \delta$ and $L + \rho_\delta$ has simple spectrum. Let $\lambda_{\delta,1} < \cdots < \lambda_{\delta,m}$ be the eigenvalues of $L + \rho_\delta$ which converge to λ as $\delta \to 0$, and let $v_{\delta,1}, \ldots, v_{\delta,m}$ be the associated eigenfunctions. Let $\lambda_{\varepsilon,\delta,j}$ be the eigenvalues of $L_\varepsilon + \rho_\delta$ which converge to $\lambda_{\delta,j}$ as $\varepsilon \to 0$. By standard elliptic estimates (Theorem 4.1), we have that there is a constant C such that $|\lambda_{\delta,j} - \lambda| \leq C\delta$, $|\lambda_{\varepsilon,\delta,j} - \lambda_{\varepsilon,j}| \leq C\delta$ and $v_{\delta,j} \to v_j$ as $\delta \to 0$, where v_j is a certain function in the eigenspace of λ. For every $\varepsilon > 0$, let us now choose the parameter δ as a function of ε, small enough so that $\delta(\varepsilon) = r(\varepsilon)$. Then, by the continuity of f, we have

$$\lambda_{\varepsilon,j} - \lambda = (\lambda_{\varepsilon,j} - \lambda_{\varepsilon,\delta(\varepsilon),j}) + (\lambda_{\varepsilon,\delta(\varepsilon),j} - \lambda_{\delta(\varepsilon),j}) + (\lambda_{\delta(\varepsilon),j} - \lambda) = f(\varepsilon, v_j) + r(\varepsilon). \tag{4.5}$$

Step 2. To retrieve the variational characterization of v_j, recall that we assumed the ordering $\lambda_{\varepsilon,1} \leq \cdots \leq \lambda_{\varepsilon,m}$ for every ε. Therefore, for $\lambda_{\varepsilon,1}$ to be the smallest eigenvalue, v_1 must be a minimizer of the right hand side of (4.5) among all eigenfunctions of λ of norm 1. Notice that if $v_{\varepsilon,j} \to v_j$ for every j, then $v_1, \dots, v_m$ must be linearly independent (since by assumption the multiplicity of λ is m). Therefore, v_2 must be the minimizer of the right hand side of (4.5) among all eigenfunctions orthonormal to v_1. Repeating the same reasoning for $\lambda_{\varepsilon,3}, \dots, \lambda_{\varepsilon,m}$, we have that (4.4) must hold for every j. □

4.2.1 Asymptotic formulae involving a bilinear function

It is useful to consider more carefully the case where the expression in the asymptotic formula admits a separation of variables as

$$f(\varepsilon, u) = E(\varepsilon) b(u, u), \tag{4.6}$$

with $b : V \times V \to \mathbb{R}$ being a symmetric bilinear form. This happens for many useful types of domain perturbations (see Section 4.3). The advantage of this case is twofold: the minimizer of (4.4) is unique and can be easily computed as follows. Choosing $u_1, \dots, u_m$ an arbitrary orthonormal basis of the eigenspace of λ, condition (4.4) can be rewritten as

$$v_n = E(\varepsilon) \operatorname{argim} \Big\{ a \cdot Ba : a \in \mathbb{R}^m,\ |a| = 1,\ a_1 u_1 + \dots + a_m u_m \perp \{v_1, \dots, v_{n-1}\} \Big\}, \tag{4.7}$$

where B is a symmetric matrix with elements

$$B_i^j = b(u_i, u_j). \tag{4.8}$$

Then, by diagonalizing B, we obtain the following result.

Corollary 4.8. If f can be rewritten as in (4.6), then the minimum and minimizer of (4.4) are respectively the n-th eigenvalue of B and $a_{1,n} u_1 + \dots + a_{m,n} u_m$, where $(a_{1,n}, \dots, a_{m,n})$ is the normalized eigenfunction of B associated to its n-th eigenvalue.

Notice that if the bilinear form b has the further decomposition

$$b(u_i, u_j) = l(u_i) l(u_j) \quad \forall i, j, \tag{4.9}$$

where $l : V \to \mathbb{R}$ is linear, an easy computation shows that the first $m-1$ eigenvalues of B are zero and the m-th one is $l(u_1)^2 + \dots + l(u_m)^2$. Therefore, we have the following result.

Corollary 4.9. If the bilinear form b can be rewritten as in (4.9), then

$$\lambda_{\varepsilon,n} - \lambda = \begin{cases} E(\varepsilon)\displaystyle\sum_{n=1}^{m} l(u_n)^2 + r(\varepsilon) & \text{if } n = m, \\ r(\varepsilon) & \text{if } n < m. \end{cases}$$

Moreover, the eigenfunction in the eigenspace of λ to which the eigenfunction of $\lambda_{\varepsilon,m}$ converges is given by

$$\frac{\sum_{n=1}^{m} l(u_n)u_n}{\sqrt{\sum_{n=1}^{m} l(u_n)^2}}.$$

4.3 Applications to eigenvalues of the Laplacian

In this section we consider some domain perturbations of particular interest in applications, and derive explicit asymptotic formulae for repeated eigenvalues of the Laplacian. Different numerical experiments are provided to validate these formulae.

4.3.1 Perturbation by a grounded inclusion

Let B be a Lipschitz domain in $\mathbb{R}^d$ with connected boundary, with volume $|B| = |\Omega|$, and centered at the origin in the sense that $\int_{\partial B} y_1 \, d\sigma(y_1, y_2) = \int_{\partial B} y_2 \, d\sigma(y_1, y_2) = 0$. Fix a point $z \in \Omega$ and consider a scaling coefficient $\varepsilon > 0$. Suppose then that the domain Ω is perturbed into $\Omega_\varepsilon = \Omega \setminus D$, by inserting an inclusion $D = z + \varepsilon B$ and requiring homogeneous Dirichlet conditions to hold on ∂D.

Let λ be an eigenvalue of Ω with associated eigenfunction u. Then λ_ε is an eigenvalue of Ω_ε perturbed from λ with associated eigenfunction u_ε if $\lambda_\varepsilon \to \lambda$ as $\varepsilon \to 0$ and

$$\begin{cases} \Delta u + \lambda u = 0 & \text{in } \Omega, \\ u = 0 \text{ or } \partial u/\partial \nu = 0 & \text{on } \partial\Omega, \end{cases} \qquad \begin{cases} \Delta u_\varepsilon + \lambda_\varepsilon u_\varepsilon = 0 & \text{in } \Omega \setminus D, \\ u_\varepsilon = 0 & \text{on } \partial D, \\ u_\varepsilon = 0 \text{ or } \partial u_\varepsilon/\nu = 0 & \text{on } \partial\Omega. \end{cases}$$

In [14, Chapter 3], the leading-order term for the perturbation of a simple eigenvalue is obtained in the case of dimensions 2 and 3. However, these computations can be repeated exactly in the same way for $d \geq 4$, and the resulting asymptotic formula can be restated as follows.

Lemma 4.10. *Given λ a simple eigenvalue of Ω with associated eigenfunction u, and λ_ε the eigenvalue of Ω_ε perturbed from λ, then*

$$\lambda_\varepsilon - \lambda = \frac{u(z)^2}{\Gamma_0(\varepsilon)} + o\left(1/\Gamma_0(\varepsilon)\right). \tag{4.10}$$

We seek to apply the variational characterization of Theorem 4.7 to our case. Assumption 4.5 holds thanks to Theorems 4.2 and 4.3, and the fact the perturbation considered is restricted to a small part of the domain. Although the expression in (4.10) is not continuous under L^2 convergence of u, we can easily rewrite it so that Assumption 4.6 holds. In fact, supposing $u_n \to u$ in L^2, we can exploit the regularity properties of solutions to elliptic equations to rewrite

$$u_n(z)^2 + o\left(1/\Gamma_0(\varepsilon)\right) = \int_{B_{r_\varepsilon}} u_n^2 \xrightarrow[n\to\infty]{} \int_{B_{r_\varepsilon}} u^2 = u(z)^2 + o\left(1/\Gamma_0(\varepsilon)\right), \tag{4.11}$$

where B_{r_ε} is a small enough ball centered at z. By Corollary 4.9, we immediately obtain the following result.

Proposition 4.11. *Let λ be an eigenvalue of multiplicity m of the negative Laplacian on Ω and $u_1, \ldots, u_m$ some associated eigenfunctions orthonormal in $\mathrm{L}^2(\Omega)$. Then, the largest perturbed eigenvalue behaves like*

$$\lambda_{\varepsilon,m} - \lambda = \frac{\sum_j u_j(z)^2}{\Gamma_0(\varepsilon)} + o\left(1/\Gamma_0(\varepsilon)\right), \tag{4.12}$$

while all the other eigenvalues behave like

$$\lambda_{\varepsilon,n} - \lambda = o(1/\Gamma_0(\varepsilon)), \qquad \textit{for } n < m.$$

Remark 4.12. We collect some interesting consequences of Proposition 4.11.

(i) For ε small enough, the largest perturbed eigenvalue $\lambda_{\varepsilon,m}$ will always be simple as long as at least one of the eigenfunctions $u_1, \ldots, u_m$ is not zero in z.

(ii) The eigenfunction associated to $\lambda_{\varepsilon,m}$ converges to

$$\frac{u_1(z)u_1 + \cdots + u_m(z)u_m}{\sqrt{u_1(z)^2 + \cdots + u_m(z)^2}}.$$

(iii) It can be shown that in two dimensions the higher-order terms in formula (4.10) can be further computed as

$$\lambda_\varepsilon - \lambda = \frac{u(z)^2}{\log(\varepsilon) + R(z)} + O\left(\varepsilon^2\right), \tag{4.13}$$

where R is a function of z which does not depend on u (see Proposition 2.9). Therefore, from Corollary 4.9, we have the better approximation

$$\lambda_{\varepsilon,n} - \lambda = \begin{cases} \dfrac{|U(z)|^2}{\log(\varepsilon) + R(z)} + O\left(\varepsilon^2\right) & \text{if } n = m, \\ \\ O\left(\varepsilon^2\right) & \text{if } n < m. \end{cases}$$

Example 4.13. Let Ω be the unit square $(0,1)^2$ and consider the Dirichlet eigenvalue $\lambda = 50\pi^2$ with associated orthonormal eigenfunctions u_1, u_2, u_3 defined as

$$\begin{cases} u_1(x,y) = 2\sin(\pi x)\sin(7\pi y), \\ u_2(x,y) = 2\sin(7\pi x)\sin(\pi y), \\ u_3(x,y) = 2\sin(5\pi x)\sin(5\pi y). \end{cases}$$

Since for any point z in Ω there is at least one eigenfunction which is non-zero at z, the insertion at z of a small grounded inclusion will cause an eigenvalue bifurcation of λ. In particular, one perturbed eigenvalue will shift from λ as $1/\log(\varepsilon)$ while the other two will shift like $O(\varepsilon^2)$. The result of a numerical simulation is presented in Figure 4.1.

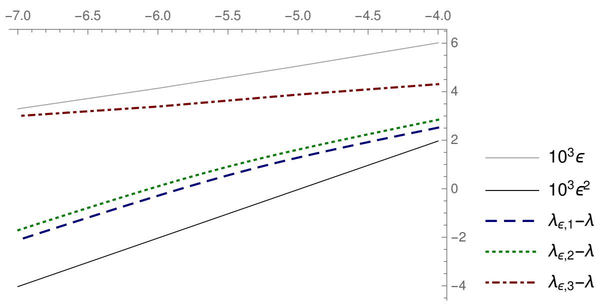


Figure 4.1: A $\log_2$-$\log_2$ plot of the behaviour of an eigenvalue bifurcation from $50\pi^2$ as the size coefficient ε of the inclusion decreases. The original domain is the unit square $(0,1)^2$ and the inclusion is a disk of radius ε centered at $(1/4, 1/4)$.

4.3.2 Perturbation by a conductivity inclusion

In this section, we consider a perturbation of Ω obtained by the insertion of a small inclusion with a conductivity coefficient different from the background.

Let B, z, ε, D be defined as in Section 4.3.1. Suppose that $-\Delta$ is perturbed into $-\Delta_\varepsilon$ by inserting inside Ω a small inclusion D of conductivity k. This causes the eigenvalue λ to split into m (possibly distinct) eigenvalues $\lambda_{\varepsilon,1} \leq \cdots \leq \lambda_{\varepsilon,m}$ such that the following system holds:

$$\begin{cases} (\Delta + \lambda_{\varepsilon,n})u_{\varepsilon,n} = 0 & \text{in } \Omega \setminus \overline{D}, \\ (k\Delta + \lambda_{\varepsilon,n})u_{\varepsilon,n} = 0 & \text{in } D, \\ u_{\varepsilon,n} \text{ continuous} & \text{along } \partial D, \\ \dfrac{\partial u_{\varepsilon,n}}{\partial \nu}\Big|_{+} = k\dfrac{\partial u_{\varepsilon,n}}{\partial \nu}\Big|_{-} & \text{on } \partial D, \\ u_{\varepsilon,n} = 0 \text{ or } \partial u_{\varepsilon,n}/\partial \nu = 0 & \text{on } \partial \Omega, \end{cases} \tag{4.14}$$

where $n = 1, \ldots, m$ and $u_{\varepsilon,n}$ are eigenfunctions associated to $\lambda_{\varepsilon,n}$.

It has been shown in [19] that if λ is a simple eigenvalue with associated eigenfunction u, and λ_ε is a perturbation of λ, then

$$\lambda_\varepsilon - \lambda = \varepsilon^d \langle \nabla u(z), \nabla u(z) \rangle_M + O(\varepsilon^{d+1}),$$

where $\langle x, y \rangle_M = x \cdot M(k, B)y$ for any $x, y \in \mathbb{R}^d$, and $M(k, B)$ is a $d \times d$ matrix known as polarization tensor, which can be defined by

$$(M(k, B))_{i,j} = \int_{\partial B} \left(\frac{k+1}{2(k-1)} I - (\mathcal{K}_B^0)^* \right)^{-1} (\nu_j) y_i \, d\sigma(y).$$

Therefore, in this case Corollary 4.8 specifies to the following result.

Proposition 4.14. *Let λ be an eigenvalue of multiplicity m of $-\Delta$ and let $u_1, \ldots, u_m$ be some associated eigenfunctions orthonormal in $\mathrm{L}^2(\Omega)$. Let $\lambda_{\varepsilon,1} \leq \cdots \leq \lambda_{\varepsilon,m}$ be the eigenvalues perturbed from λ which are solutions to (4.14). Then, for every $n \in \{1, \ldots, m\}$, the $O(\varepsilon^{d+1})$ approximation of $\lambda_{\varepsilon,n} - \lambda$ is given by the n-th eigenvalue of the matrix with element*

$$\varepsilon^d \langle \nabla u_i(z), \nabla u_j(z) \rangle_M$$

in position (i, j).

Remark 4.15. We consider some extremal cases of Proposition 4.14 that are of particular interest.

(i) If $\langle \nabla u_i(z), \nabla u_j(z) \rangle_M = 0$ for all $i \neq j$, then it is enough to reorder $u_1, \ldots, u_m$ according to the magnitude of $\langle \nabla u_1(z), \nabla u_1(z) \rangle_M, \ldots, \langle \nabla u_m(z), \nabla u_m(z) \rangle_M$, to obtain that for any n it holds

$$\lambda_{\varepsilon,n} - \lambda = \varepsilon^d \langle \nabla u_n(z), \nabla u_n(z) \rangle_M + O(\varepsilon^{d+1}).$$

We also remark that if the multiplicity m is larger than the dimension d, only d vectors can be linearly independent, and thus we will have that $\lambda_{\varepsilon,n} - \lambda = O(\varepsilon^{d+1})$ for $n \leq m - d$.

(ii) If $\nabla u_i(z), \nabla u_j(z)$ are parallel with respect to $\langle \cdot, \cdot \rangle_M$, then, by Corollary 4.9, we will have

$$\lambda_{\varepsilon,n} - \lambda = \begin{cases} \varepsilon^d \sum_{n=1}^m \langle \nabla u_n(z), \nabla u_n(z) \rangle_M + O\left(\varepsilon^{d+1}\right) & \text{if } n = m, \\ \\ O\left(\varepsilon^{d+1}\right) & \text{if } n < m. \end{cases}$$

Example 4.16. Let Ω be the unit square $(0,1)^2$ and consider the Neumann eigenvalue $\lambda = 100\pi^2$ with associated eigenfunctions u_1, u_2, u_3, u_4 defined as

$$\begin{cases} u_1(x,y) = \sqrt{2}\cos(10\pi y), \\ u_2(x,y) = \sqrt{2}\cos(10\pi x), \\ u_3(x,y) = 2\cos(6\pi x)\cos(8\pi y), \\ u_4(x,y) = 2\cos(8\pi x)\cos(6\pi y). \end{cases}$$

Let B be the disk of radius $1/\pi^2$ centered at 0. In this case, it can be explicitly computed that $M(k,B) = 2(k-1)I/(\pi^2(k+1))$. We can easily determine, reasoning as in Remark 4.15, whether the first term in the asymptotic expansion of $\lambda_{\varepsilon,n} - \lambda$ is zero; such behaviour will depend on the choice of z. For example:

- for $z = (1/2, 1/2)$, it holds $\nabla u_n(z) = 0$ for any n, and therefore $\lambda_{\varepsilon,n} - \lambda = O(\varepsilon^3)$;

- for $z = (1/3, 1/2)$, $\nabla u_1(z) = \nabla u_3(z) = 0$ while $\nabla u_2(z), \nabla u_4(z)$ are all parallel and non-zero, thus from Item ii of Remark 4.15 we have $\lambda_{\varepsilon,n} - \lambda = O(\varepsilon^3)$ for $n = 1, 2, 3$ while $\lambda_{\varepsilon,4} - \lambda = \Theta(\varepsilon^2)$;

- for $z = (1/7, 1/7)$ computations of the gradient of the eigenfunctions at z show that $\lambda_{\varepsilon,n} - \lambda = O(\varepsilon^3)$ for $n = 1, 2$ and $\lambda_{\varepsilon,n} - \lambda = \Theta(\varepsilon^2)$ for $n = 3, 4$;

- by Item i of Remark 4.15 there is no $z \in \Omega$ such that $\lambda_{\varepsilon,n} - \lambda = \Theta(\varepsilon^2)$ for more than two different indices n.

Example 4.17. Let Ω be the unit square $(0,1)^2$ and consider the Neumann eigenvalue $\lambda = 4\pi^2$ with associated eigenfunctions u_1, u_2 defined as

$$\begin{cases} u_1(x,y) = \sqrt{2}\cos(2\pi y), \\ u_2(x,y) = \sqrt{2}\cos(2\pi x). \end{cases}$$

Let B be the disk of radius $1/\pi^2$ centered at 0. Recall that in this case we have $M(k,B) = 2(k-1)I/(\pi^2(k+1))$. Although the first term in the asymptotic formula for $\lambda_{\varepsilon,n} - \lambda$ can be easily computed in this case, here we focus our attention only on the asymptotic order. We can easily determine, reasoning as in Remark 4.15, whether the first term in the asymptotic expansion of $\lambda_{\varepsilon,n} - \lambda$ is zero; such behaviour will depend on the choice of z. For example:

- for $z = (1/2, 1/2)$, we have that both eigenfunctions u_1, u_2 have zero gradient at 0, and thus both eigenvalues shift from λ as $O(\varepsilon^3)$;
- for $z = (1/4, 1/2)$, one of the eigenfunctions has zero gradient while the other has a non-zero entry, thus one eigenvalue shift behaves like ε^2, the other like $O(\varepsilon^3)$;
- for $z = (1/4, 1/4)$, the gradients of the two eigenfunctions are orthogonal and non-zero, thus both eigenvalues shift from λ as ε^2.

Numerical results are presented in Figure 4.2.

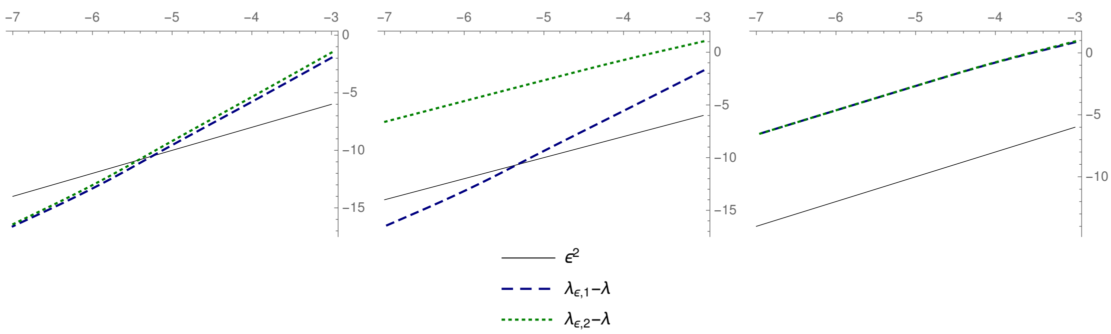


Figure 4.2: A $\log_2$-$\log_2$ plot of the behaviour of an eigenvalue bifurcation as the size coefficient ε of the conductivity inclusion decreases. The original domain is the unit square $(0,1)^2$, the inclusion a disk of conductivity $k = 2$, centered respectively at $(1/2, 1/2)$ (left graph), at $(1/4, 1/2)$ (center graph), at $(1/4, 1/4)$ (right graph).

4.3.3 Perturbation by boundary deformation

In this section, we consider Ω_ε obtained from Ω by a boundary deformation. For simplicity, we suppose that Ω is globally the epigraph of a Lipschitz function φ, that is $\Omega = \big\{x \in \mathbb{R}^d : \varphi(x) \le 0\big\}$. Given $w \in \mathrm{C}^2(\partial\Omega)$, we also suppose that the boundary perturbation is such that $\Omega_\varepsilon = \{x \in \mathbb{R}^d : \varphi(x) + \varepsilon w(x)\nu(x) \le 0\}$. Recall that if λ is a simple eigenvalue of Ω with associated eigenfunction u, and $\lambda_\varepsilon \to \lambda$, then Hadamard's formula reads

$$\frac{\partial \lambda_\varepsilon}{\partial \varepsilon}\Big|_{\varepsilon=0} = \int_{\partial\Omega} \Big(|\nabla u|^2 - \lambda u^2 - 2(\partial u/\partial \nu)^2\Big) w, \tag{4.15}$$

for Dirichlet or Neumann conditions on $\partial\Omega$ (for its proof see [28] or [51]). Therefore, if λ has multiplicity m, an application of Theorem 4.7 provides us with the variational formula

$$\lambda_{\varepsilon,n} - \lambda = \varepsilon \operatorname*{argim}_{v \in S_n} \int_{\partial\Omega} \Big(|\nabla v|^2 - \lambda v^2 - 2(\partial v/\partial \nu)^2\Big) w + O(\varepsilon^2). \tag{4.16}$$

Example 4.18. Let $\Omega = (0,1)^2$ and consider the Dirichlet eigenvalue $\lambda = 10\pi^2$ with associated orthonormal eigenfunctions $u_1(x,y) = 2\sin(\pi x)\sin(3\pi y)$, $u_2(x,y) = 2\sin(3\pi x)\sin(\pi y)$. Suppose that the boundary of Ω is perturbed on the upper side of the square Ω with $w(x,y) = \sin(\pi x)$, that is $\partial\Omega \cap \{y = 1\}$ is deformed into $\{(x,y) : 0 \le x \le 1, y = 1 + \varepsilon \sin(\pi x)\}$. In this case, the integral in (4.15) is analytically computable as

$$-\int_{\partial\Omega} (a_1 \partial u_1/\partial \nu + a_2 \partial u_2/\partial \nu)^2 w = \frac{16\pi}{35}(-105a_1^2 + 14a_1a_2 - 9a_2^2).$$

Thus, by (4.16), we can calculate explicitly

$$\begin{aligned} u_{\varepsilon,1} &\to c_1u_1 + c_2u_2, & \lambda_{\varepsilon,1} - \lambda &= C_1\varepsilon + O(\varepsilon^2), \\ u_{\varepsilon,2} &\to c_2u_1 - c_1u_2, & \lambda_{\varepsilon,2} - \lambda &= C_2\varepsilon + O(\varepsilon^2), \end{aligned} \tag{4.17}$$

where $c_1 \simeq 0.997, c_2 \simeq -0.0724, C_1 \simeq -152, C_2 \simeq -12.2$. Numerical results are presented in Figures 4.3 and 4.4.

Notice that in general, minimizing the expression in (4.16) is a computationally expensive task. However, we can still obtain some cheaper, qualitative information if we approximate to a more treatable form the considered domain perturbation. We showcase such an heuristic in the following example, where a local perturbation is "singularized" to obtain an asymptotic formula easier to analyze.

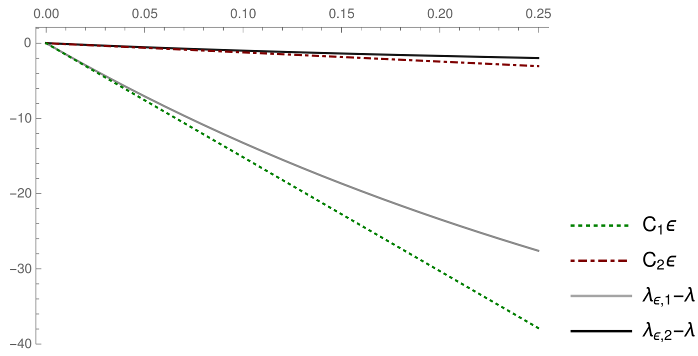


Figure 4.3: Behaviour of an eigenvalue bifurcation as the scaling parameter ε of the boundary deformation decreases. The original domain is the unit square $(0,1)^2$ and the boundary deformation is given by $\varepsilon \sin(\pi x)\nu(x,1)$ on the upper side.

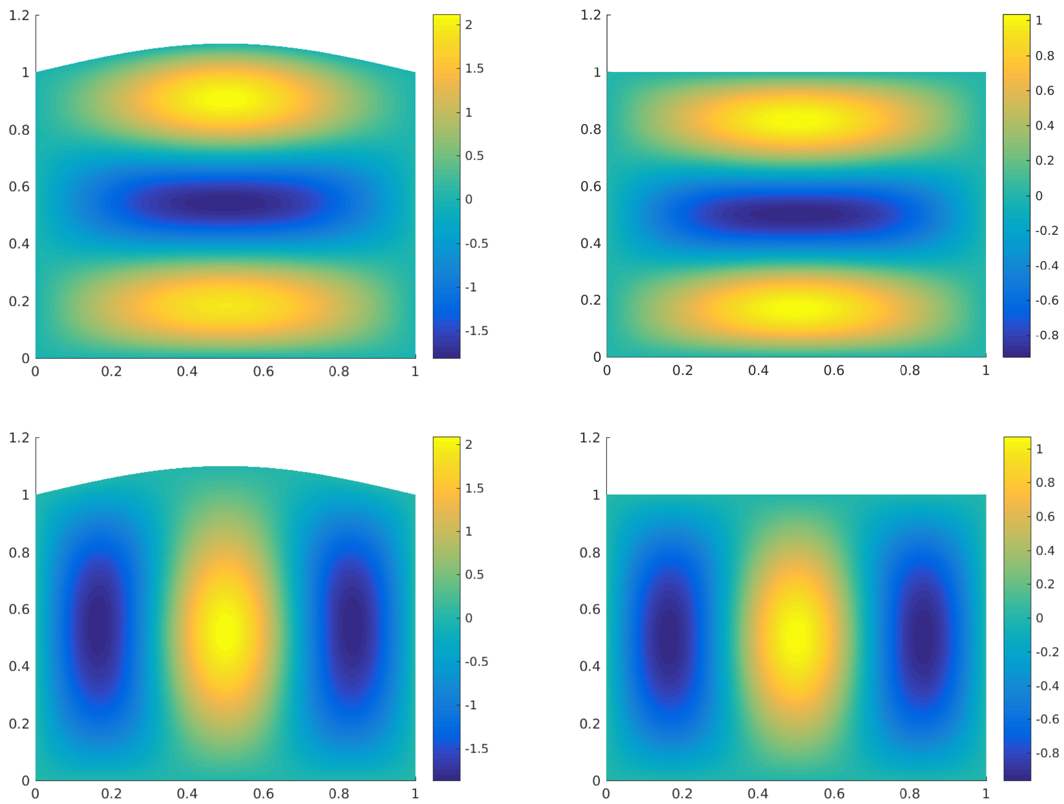


Figure 4.4: Eigenfunctions associated to the eigenvalues perturbed from $10\pi^2$. The perturbation consists in a boundary deformation $\varepsilon \sin(\pi x)\nu(x,1)$ of the upper side for $\varepsilon = 1/10$. Numerical computations obtained with the finite element method of the eigenfunctions are plotted in the left column, their limiting functions as $\varepsilon \to 0$ in the two-dimensional eigenspace of $4\pi^2$ given by (4.17) in the right column.

Example 4.19. Suppose a small dent is present on the surface $\partial\Omega$ at the point z, shaped as a cone with circular base of radius δ and height ε. Let at first λ be a simple Dirichlet eigenvalue with associated eigenfunction u. If we approximate

$$\int_{\partial\Omega} (\partial u/\partial\nu)^2 w \simeq \delta^2\pi(\partial u(z)/\partial\nu)^2,$$

then for eigenvalues low enough we can estimate

$$\lambda_\varepsilon - \lambda \simeq -\varepsilon\delta^2\pi(\partial u(z)/\partial\nu)^2. \tag{4.18}$$

The right hand side in (4.18) is bilinear in u therefore, if we adopt such an approximation for $\lambda_\varepsilon - \lambda$, by Corollary 4.9 we have that for any non-simple eigenvalue the largest perturbed eigenvalue will shift like $O(\varepsilon)$ while all the smaller ones will shift like $O(\varepsilon^2)$.

4.3.4 Summary of results

We summarize hereafter the main results obtained for each of the perturbations considered. For this purpose, we recall that Ω indicates an arbitrary Lipschitz domain in $\mathbb{R}^d$, λ an eigenvalue of the negative (Dirichlet or Neumann) Laplacian on Ω, $u_1, \dots, u_m$ an arbitrary orthonormal basis in $\mathrm{L}^2(\Omega)$ of the eigenspace of λ, and $\lambda_{\varepsilon,1} \le \cdots \le \lambda_{\varepsilon,m}$ the eigenvalues perturbed from λ.

- When a hole D of volume ε^d and centered at z is cut out from Ω and homogeneous Dirichlet boundary conditions are imposed on ∂D, we have

  $$\begin{aligned} \lambda_{\varepsilon,m} - \lambda &= C\varepsilon^{d-1}\sum_{i=1}^m u_i(z)^2 + O(\varepsilon^d), \\ \lambda_{\varepsilon,n} - \lambda &= O(\varepsilon^d) \qquad \text{for } n < m, \end{aligned}$$

  in the case where $d \ge 3$ (see (4.13) for the case $d = 2$), where C is a constant which depends only on the dimension d. Therefore, we have that the largest eigenvalue splits at a higher asymptotic order than all the others eigenvalues, as long as one among the quantities $u_1(z), \dots, u_m(z)$ is non-zero.

- In the case of a conductivity inclusion, we do not have such an explicit formula, but we can still easily recover a first-order approximation by computing the eigenvalues of a finite matrix. More precisely, if we suppose to change the conductivity coefficient from 1 to k only in D, a small disk of radius ε centered at a point z, then for any $n \in \{1, \ldots, m\}$,

$$\lambda_{\varepsilon,n} - \lambda \; = 2\frac{k-1}{k+1}\varepsilon^d \mu_n + O(\varepsilon^{d+1}),$$

where μ_n is the n-th eigenvalue of the matrix with element $\nabla u_i(z) \cdot \nabla u_j(z)$ in position (i, j).

- In the case of a normal boundary deformation of Ω with shape $w \in \mathrm{C}^2(\partial\Omega)$, that is the perturbed domain boundary is given locally by $\partial\Omega + \varepsilon w \nu$, to find $\lambda_{\varepsilon,n} - \lambda$ for any $n \in \{1, \ldots, m\}$, one has to find the minimizer v_n of

$$J(v) = \int_{\partial\Omega} \Big(|\nabla v|^2 - \lambda v^2 - 2(\partial v/\partial \nu)^2 \Big) w,$$

among all v's of unit L^2-norm in the eigenspace of λ and perpendicular to $v_1, \ldots, v_{n-1}$. Then

$$\lambda_{\varepsilon,n} - \lambda = \varepsilon J(v_n).$$

As a final remark, let us point out that similar formulae can be derived for many other types of domain perturbations or other differential operators. For example, with the same approach of Section 4.3.3, it is immediate to generalize the asymptotic expansion of eigenvalues in the case of shape deformation of conductivity inclusions (see [3, Theorem 2.1]); or, with the same approach of Section 4.3.2, to generalize the asymptotic formulae for eigenvalues of the Lamé operator in the context of linear elasticity (see [4, Theorem 2.1]).

Chapter 5

Reconstruction of small perturbations from eigenvalues' shifts

A foundational question in spectral geometry is whether the eigenvalues of a differential operator characterize the shape of the domain on which it is defined. Although in general the answer is negative, in many special cases of interest the answer is affirmative (for instance, a square is uniquely characterized by its first Dirichlet or Neumann Laplacian eigenvalue). In this chapter we try to devise some practical procedures to reconstruct a domain from its eigenvalues under some restricting assumptions. More precisely, we suppose that our unknown domain is given by a small perturbation from a known domain, that the perturbation is completely characterized by some parameters, and that we intend to estimate these parameters from the knowledge of the eigenvalues of both the known and the unknown domain.

More formally, let Ω be a domain and let $(\lambda_j)_{j\in\mathbb{N}}$ be the sequence of eigenvalues of the negative Laplacian on Ω with Dirichlet or Neumann boundary conditions. Consider the first N different eigenvalues of Ω,

$$\lambda_1 = \cdots = \lambda_{M_1} < \lambda_{M_1+1} = \cdots = \lambda_{M_2} < \cdots < \lambda_{M_{n-1}+1} = \cdots = \lambda_{M_N},$$

where $M_j = m_1 + \cdots + m_j$ and m_j is the multiplicity of λ_j. Let u_j indicate an eigenfunction associated to λ_j, and suppose that $u_1, \ldots, u_{M_N}$ are orthonormal in $L^2(\Omega)$.

Suppose now that Ω is perturbed into another domain Ω_ε. We write down the perturbed eigenvalues of Ω_ε as

$$\lambda_{\varepsilon,1} \leq \cdots \leq \lambda_{\varepsilon,M_1} < \lambda_{\varepsilon,M_1+1} \leq \cdots \leq \lambda_{\varepsilon,M_2} < \cdots < \lambda_{\varepsilon,M_{n-1}+1} \leq \cdots \leq \lambda_{\varepsilon,M_N},$$

and suppose that the perturbation is small enough so that there is no eigenvalue crossing, i.e., $\lambda_{\varepsilon,j} \to \lambda_j$ as $\varepsilon \to 0$ for $j = 1, \ldots, M_N$. In this chapter, we show how to reconstruct some features of Ω_ε, via the asymptotic formulae derived in the previous chapters, from the knowledge of Ω, of $\lambda_1, \ldots, \lambda_N$ and of $\lambda_{\varepsilon,1}, \ldots, \lambda_{\varepsilon,N}$. We consider three types of domain perturbations: grounded inclusions, conductivity inclusions, and boundary deformations.

5.1 Grounded inclusion

In this section we assume that the perturbation is caused by a grounded inclusion, that is $\Omega_\varepsilon = \Omega \setminus \overline{D}$ where $D = z + \varepsilon B$ and homogeneous Dirichlet boundary conditions are imposed on ∂D.

Direct problem. Let

$$U_j(z) = \begin{cases} (u_{M_{k-1}+1}(z), \ldots, u_{M_k}(z)) & \text{if } j = M_k \text{ for some } k, \\ 0 & \text{otherwise.} \end{cases} \tag{5.1}$$

From (4.13), we know that

$$\lambda_{\varepsilon,j} - \lambda_j = \mathfrak{c}(B) \frac{|U_j(z)|^2}{\Gamma_0(\varepsilon)} + o(1/\Gamma_0(\varepsilon)), \tag{5.2}$$

where

$$\mathfrak{c}(B) = \begin{cases} \operatorname{cap}(\partial B) & d \geq 3, \\ 1 & d = 2. \end{cases} \tag{5.3}$$

In two dimensions, this approximation is sometimes too poor for our purposes due to the slow convergence to 0 of $1/\log(\varepsilon)$ as $\varepsilon \to 0$. In this case, we can use the more accurate, although more computationally expensive, asymptotic expression

$$\lambda_{\varepsilon,j} - \lambda_j = \frac{|U_j(z)|^2}{\Gamma_0(\varepsilon \sqrt{\lambda_j} \operatorname{cap}(\partial B) \eta_0) + \mathfrak{r}(z)} + O(\varepsilon^2), \tag{5.4}$$

where $\mathfrak{r}$ is defined in (2.7).

Inverse problem. Our inverse problem is to reconstruct ε, z and the capacity $\operatorname{cap}(\partial B)$ from the knowledge of $\lambda_{\varepsilon,M_k}$ and λ_{M_k} for $k = 1, \ldots, M_N$. We will proceed in several steps, assuming the knowledge of some of these quantities to recover the others.

Notice that in the case of an eigenvalue with multiplicity $m_k > 1$, only the largest perturbation is of order $O(1/\Gamma_0(\varepsilon))$ while all the others are of higher order; so only the eigenvalues $\lambda_{\varepsilon,M_k}$ and λ_{M_k} will be used for the purposes of inclusion reconstruction.

Size reconstruction. Assume at first that $\mathfrak{c}(B)$ is known. If homogeneous Neumann conditions are imposed on $\partial\Omega$, an estimate on the size of the inclusion can be obtained immediately from the first eigenvalue shift; in fact in this case we know that $\lambda_1 = 0$ is simple and $u_1^2 \equiv 1/|\Omega|$. Thus, from (5.2), we immediately have the approximation

$$\varepsilon \simeq \Gamma_0^{-1}\big(\mathfrak{c}(B)/(|\Omega|\lambda_{\varepsilon,1})\big). \tag{5.5}$$

This estimate is sometimes not accurate enough, especially in two dimensions.

Let us assume that the position z is also known. Then we can obtain an improved approximation by considering multiple eigenvalues and looking for a minimizer of the discrepancy function (obtained from (5.2))

$$\delta \mapsto \sum_{j=1}^{N} \big(\lambda_{\varepsilon,j} - \lambda_j - \mathfrak{c}(B)|U_j(z)|^2/\Gamma_0(\delta)\big)^2, \tag{5.6}$$

or, in two dimensions, for a minimizer of

$$\delta \mapsto \sum_{j=1}^{N} \left(\lambda_{\varepsilon,j} - \lambda_j - \frac{|U_j(z)|^2}{\Gamma_0(\delta\sqrt{\lambda_j}\operatorname{cap}(\partial B)\eta_0) + R_j(z)}\right)^2. \tag{5.7}$$

We remark that both the last two approaches are viable also under homogeneous Dirichlet boundary conditions on $\partial\Omega$.

Example 5.1. Consider the case where $\Omega = B \subseteq \mathbb{R}^2$ is the unit disk and Neumann boundary conditions are imposed on $\partial\Omega$. We want to reconstruct the size coefficient ε from the knowledge of some eigenvalues' shifts and the position z. A reconstruction based only on the shift of the first eigenvalue through formula (5.5) is presented in Figure 5.1. The values obtained from the asymptotic formulae are confronted with the accurate estimates given by the multipole expansion method. A reconstruction of ε via the minimization of (5.6) and (5.7), known the perturbation of the first five eigenvalues, are presented respectivelty in Figures 5.2 and 5.3. Notice how the reconstruction via the more computationally expensive formula (5.7) is more accurate, especially when the center z of the perturbation is near the boundary of Ω, compared to the reconstruction via (5.6) or (5.5).

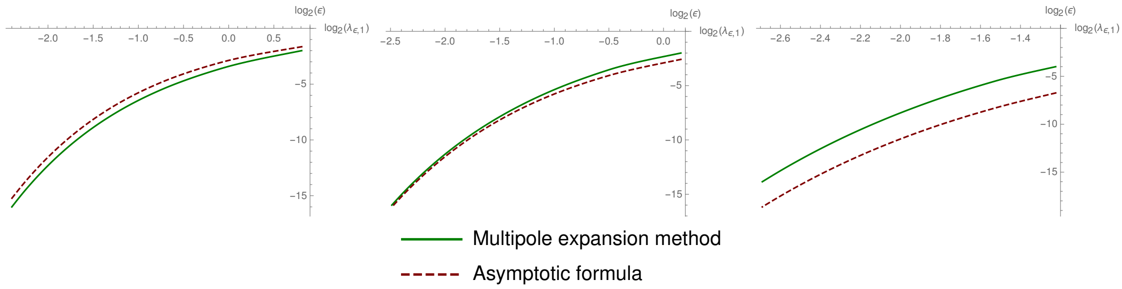


Figure 5.1: A log-log plot of ε as a function of $\lambda_{\varepsilon,1}$ for different choices of z (from left to right, $|z| = .3, .6, .9$).

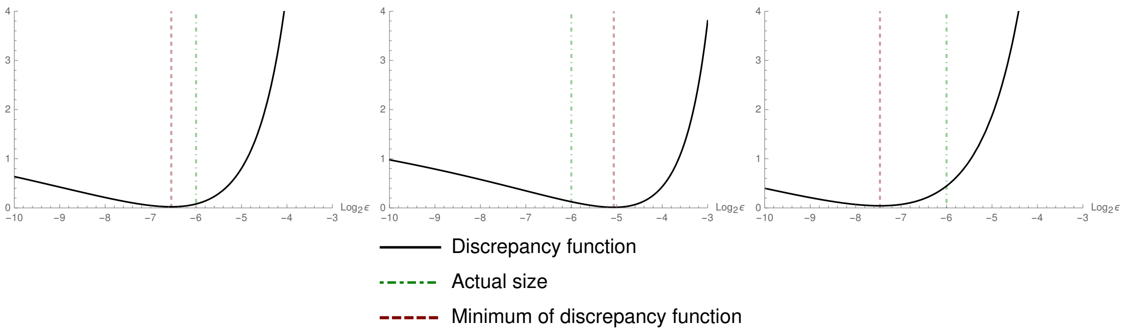


Figure 5.2: A plot of the the discrepancy function (5.6) with $N = 5$ and $|\varepsilon| = 2^{-6}$ for different choices of z (from left to right $|z| = .3, .6, .9$).

Position reconstruction. Suppose that the size ε and the capacity $\mathrm{cap}(\partial B)$ are known. A position estimate can be obtained by searching for a z which satisfies (5.2). An important warning in this case is that there is no guarantee of uniqueness. In fact, from a single eigenvalue shift one can obtain at most all the points which lie on the same level set of $|U_j|^2$. A possible solution to this problem would be to take many eigenvalue shifts, thus restricting significantly the possible values which z can take. More specifically, one hopes that the intersection of the level sets of different eigenfunctions becomes a point if we consider enough eigenfunctions. Although

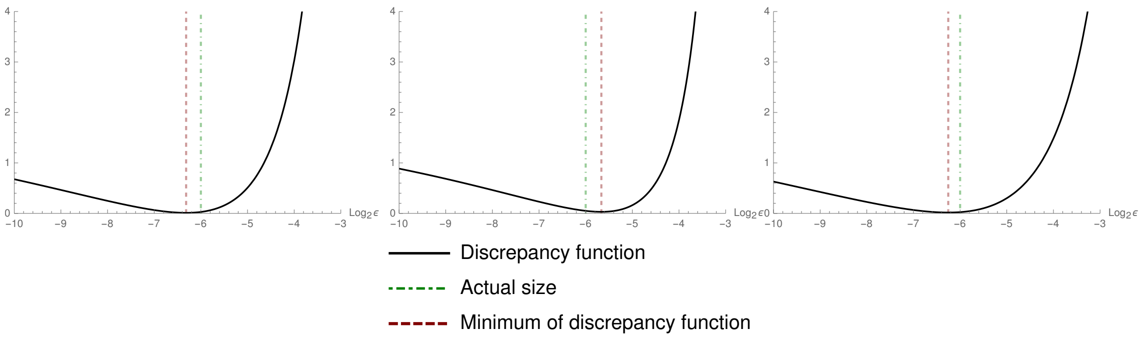


Figure 5.3: A plot of the the discrepancy function (5.7) with $N = 5$ and $|\varepsilon| = 2^{-6}$ for different choices of z (from left to right, $|z| = .3, .6, .9$).

this might be true for some non-symmetric domains, it is false for domains which present some symmetries. However, as is shown in the following examples, we can still recover some useful information even in the case of a symmetric domain.

Example 5.2 (Ball or spherical shell domain). Let $\Omega \subseteq \mathbb{R}^d$ be a ball or a spherical shell (that is the set difference of two concentric balls of different radii). In this case, the Neumann eigenfunctions of Ω can be written by separation of variables as a product of a radial and an angular part. Then, although we can not recover z univocally, we can recover its distance from the origin $|z|$ from the shift of the first non-zero eigenvalue of Ω. In fact, the first non-zero Neumann eigenvalue of the ball has associated eigenfunctions $u_2, \ldots, u_{d+1}$ such that $|U_2(x)|^2 = u_2(x)^2 + \cdots + u_{d+1}(x)^2 = CR(|x|)$, where C is a constant and R a bijective function. Therefore, from (5.2) we can recover a first-order approximation of $|z|$. Notice that the dependence on only the distance from the center of the squared eigenfunction actually holds for any eigenfunction, that is, for any j, a constant C_j and a function R_j can be found such that $|U_j(x)|^2 = C_j R_j(|x|)$. Therefore, the knowledge of more eigenvalues' shifts does not give us any additional information on z. This can be seen also as an immediate consequence of the fact that a ball with a hole at z is isometric to a ball with the same hole at x for any $|x| = |z|$.

Example 5.3 (Cubic domain). Let $\Omega = (0, \pi)^d$ be a d-dimensional cube. It is well known that the Neumann eigenfunctions and eigenvalues of Ω are given respectively by $\cos(n_1 x_1) \ldots \cos(n_d x_d)$ and $n_1^2 + \cdots + n_d^2$ for $n_1, \ldots, n_d$ non-negative integers. Therefore, if we know the shift of the first non-zero eigenvalue, that is 1, we can recover from (5.2) the quantity $f(z) = \cos(z_1)^2 + \cdots + \cos(z_d)^2$. If we also know the shift of the second non-zero eigenvalue, that is 4, we can recover $g(z) = \cos(2z_1)^2 + \cdots + \cos(2z_d)^2$. It can be shown that any two level sets of f and g intersect at most at $d2^d$ points, where each point is the image through a reflection along a symmetry hyperplane of the cube (some of these points might coincide when z lies on a symmetry hyperplane of Ω); see Figure 5.4 for a plot of the level sets of squared eigenfunctions in the two dimensional case. Since we know that such domains are

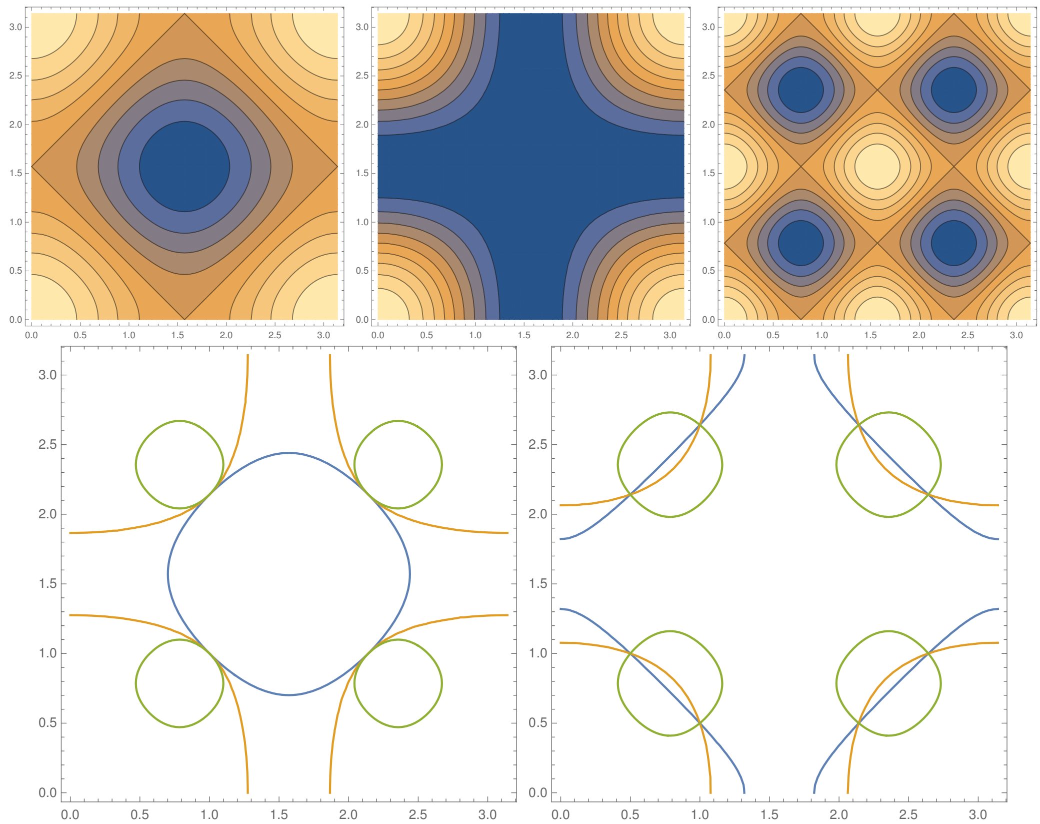


Figure 5.4: Level sets of squared eigenfunctions.

isometric, using more eigenvalues won't give us any additional information on the position z.

Capacity and shape reconstruction. If the size coefficient ε and position z are known, then the capacity $\mathrm{cap}(\partial B)$ can be recovered by inverting (5.2). The capacity can be useful to determine the shape of an inclusion, if we know a priori that it belongs to a certain class of shapes, like for instance in the following example.

Example 5.4. Let $B \subseteq \mathbb{R}^2$ be an ellipse of semi-axes a_1, a_2 such that $a_1 a_2 = 1$. Then $\mathrm{cap}\, \partial B = (a_1 + 1/a_1)/2$. From the knowledge of ε and z, an estimate of a_1 can then be obtained by using (5.2). A numerical computation of a_1 as a function of $\lambda_{\varepsilon,1} - \lambda_1$ in the case of Ω a disk of radius 1 and Dirichlet boundary conditions on $\partial\Omega$ is given in Figure 5.5.

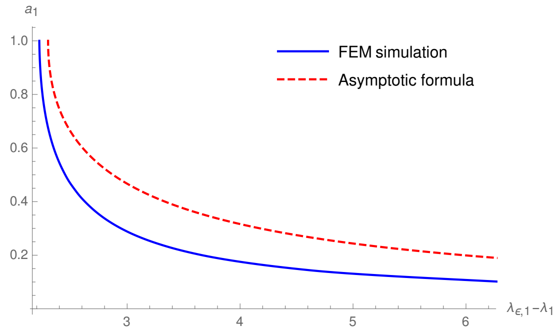


Figure 5.5: Semi-axis length of an elliptic inclusion as a function of an eigenvalue shift.

Even if in most cases we can not determine univocally the shape of the inclusion from its capacity, we can at least reduce the dimension of the parameter space which describes its shape.

Example 5.5. Let $B \subseteq \mathbb{R}^3$ be an ellipsoid of semi-axes a_1, a_2, a_3 such that $4/3\pi a_1 a_2 a_3 = 1$. Then by [56, p. 156],

$$\frac{1}{\operatorname{cap} \partial B} = 2\pi \int_0^\infty \frac{dx}{\sqrt{a_1^2 + x}\sqrt{a_2^2 + x}\sqrt{(3/(4\pi a_1 a_2))^2 + x}}. \tag{5.8}$$

Therefore, level curves (see Figure 5.6) of the integral in the previous equation seen as a function of a_1, a_2 will represent the continuous class of ellipsoids with area 1 which cause a given eigenvalue perturbation.

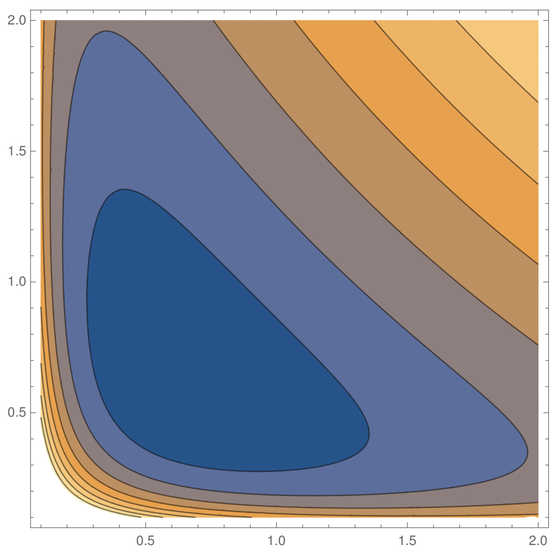


Figure 5.6: level curves of the integral in (5.8)

General reconstruction. If the capacity is known, the size and position can be estimated from the knowledge of only two eigenvalues as follows. By considering the ratio of the perturbations, one can estimate the position looking for the level sets of the ratio of squared eigenfunction. Then, ε can be found by backsubstituting the value of the eigenfunction estimated at z.

The case where the size, position and capacity are unknown and have to be reconstructed from the eigenvalue perturbation is much more delicate. There may be multiple classes of inclusions with different size, position and shape which cause a certain eigenvalue perturbation. If some a priori information on these features is known, the search in the parameter space can be limited, as has been done in the previously considered cases, but a general approach does not appear to be viable.

5.2 Conductivity inhomogeneity

In this section, we suppose that the perturbation is caused by a conductivity inclusion, that is, $\Omega_\varepsilon = \Omega \setminus \overline{D}$ with $D = z + \varepsilon B$ and $k \neq 1$ being the conductivity of D.

Direct problem. In this case, the perturbed eigenvalues satisfy the system

$$\begin{cases} (\Delta + \lambda_{\varepsilon,n})u_{\varepsilon,n} = 0 & \text{in } \Omega \setminus \overline{D}, \\ (k\Delta + \lambda_{\varepsilon,n})u_{\varepsilon,n} = 0 & \text{in } D, \\ u_{\varepsilon,n} \text{ continuous} & \text{along } \partial D, \\ \dfrac{\partial u_{\varepsilon,n}}{\partial \nu}\Big|_{+} = k\dfrac{\partial u_{\varepsilon,n}}{\partial \nu}\Big|_{-} & \text{on } \partial D, \\ u_{\varepsilon,n} = 0 \text{ or } \partial u_{\varepsilon,n}/\partial\nu = 0 & \text{on } \partial\Omega. \end{cases} \tag{5.9}$$

From Proposition 4.14, we have the asymptotic expansion

$$\lambda_{\varepsilon,j} - \lambda_j = \varepsilon^d \mu_j + O(\varepsilon^{d+1}), \tag{5.10}$$

where μ_j is the j-th eigenvalue of the matrix

$$\Big(\nabla u_p(z) \cdot M(k,B)\nabla u_q(z)\Big)_{p=M_{j-1}+1,\dots,M_j}^{q=M_{j-1}+1,\dots,M_j}, \tag{5.11}$$

with $M(k,B)$ being the polarization tensor matrix (see (1.12)). We consider hereafter the reconstruction of different features of the conductivity inclusion.

Size reconstruction. Suppose that the position and the polarization tensor of B are known. Then the problem of reconstructing the size coefficient ε, as in Section 5.1, can be solved directly by inverting (5.10). In the same way, a finer estimate can be obtained by minimizing a discrepancy functional which takes into account the perturbation of more than one eigenvalue.

Position reconstruction. Suppose that the size coefficient ε and the polarization tensor of B are known. Then, we can reconstruct the position z by looking at the level sets of $\nabla U \cdot M \nabla U$.

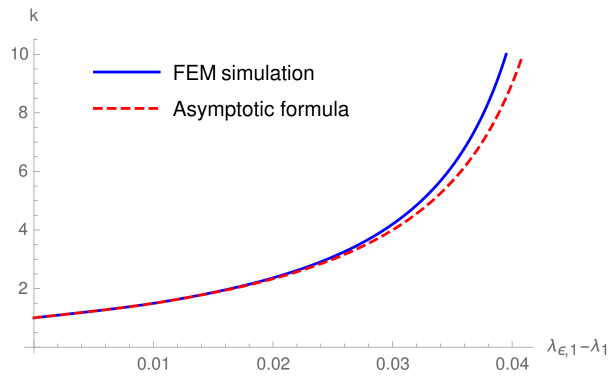
Example 5.6. Let $\Omega = B \subseteq \mathbb{R}^2$ be the unit disk. It is known that the polarization tensor is $M = 2(k-1)I/(k+1)$. Therefore, in this case we need to look for intersections of levels sets of the squared norm of the gradient of the eigenfunctions. Since they are radially symmetric, we can reconstruct the distance of the particle from the center.

Polarization tensor, conductivity and shape reconstructions. We can reconstruct the polarization tensor using formula (5.10) for different frequencies $\lambda_{\varepsilon,1}, \dots,$ $\lambda_{\varepsilon,M_N}$ and looking for a $d \times d$ matrix which minimizes the discrepancy.

If we know a priori the shape of the inclusion B, we can directly reconstruct its conductivity, as is done in the following simple example.

Example 5.7. Suppose that $\Omega = B \subseteq \mathbb{R}^2$ is the unit disk and suppose that we are interested in reconstructing the conductivity k of B. Fix the size coefficient $\varepsilon = 0.1$ and the center of B in $(0.3, 0)$. A plot of k as a function of the eigenvalue shift is given in Figure 5.7.

Figure 5.7: Conductivity as a function of the first eigenvalue shift.



5.3 Boundary deformation

In this final section, we suppose only the boundary of the domain is deformed, and try to reconstruct some characterizing features.

Direct problem. Let $\phi(t,x) : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ be such that $\phi(0,x) = x$ for any $x \in \mathbb{R}^d$ and let $\phi(t,\Omega)$ be diffeomorphic to Ω for any t. Let $\lambda(t)$ be a simple Dirichlet eigenvalue of $\phi(t,\Omega)$. Then, from (3.5), we have that

$$\dot{\lambda}(t) = -\int_{\phi(t,\partial\Omega)} (\partial u(t,y)/\partial\nu(t,y))^2 \dot{e}(t,y)\cdot\nu(t,y)\, d\sigma(y), \tag{5.12}$$

where $u(t,\cdot)$ is the L^2-normalized eigenfunction of $\phi(t,\Omega)$ associated to $\lambda(t)$, $\nu(t,\cdot)$ is the outward normal to the surface $\phi(t,\partial\Omega)$, $e(t,\cdot)$ is the identity on $\phi(t,\partial\Omega)$. By a change of variable,

$$\dot{\lambda}(t) = -\int_{\partial\Omega} (\partial u(t,\phi(t,x))/\partial\eta(t,x))^2 \dot{\phi}(t,x)\cdot\eta(t,x) G(t,x), \tag{5.13}$$

where G is the absolute value of the determinant of the Gramian of ϕ and $\eta(t,x) = \nu(t,\phi(t,x))$.

If w is a smooth function defined on $\partial\Omega$ such that

$$\phi(t,x) = x + tw(x)\nu(0,x) \qquad \forall x \in \partial\Omega, \tag{5.14}$$

then (5.13) simplifies to

$$\dot{\lambda}(0) = -\int_{\partial\Omega} (\partial u/\partial\eta)^2 w\, d\sigma(x), \tag{5.15}$$

where $u, \eta, \dot{\eta}, G$ are assumed to be functions of $(0,x)$, and w to be function of x. We are interested in using this first-order asymptotic formula to reconstruct the magnitude of the boundary deformation.

Inverse problem. We consider two simple examples of boundary deformation reconstruction which are of interest in applications.

Example 5.8 (Deformation of a side of a rectangle). Consider the rectangle $\Omega = [0,1] \times [-l,0]$. Suppose for now that l is irrational, so that all eigenvalues of Ω are simple. More precisely, we have that the L^2-normalized Dirichlet eigenfunctions of Ω are given by

$$u_{n,m}(x,y) = \frac{1}{4}\sin(n\pi x)\sin(m\pi y/l),$$

and the associated eigenvalues by $\lambda_{n,m}(0) = (n\pi)^2 + (m\pi/l)^2$, for n, m positive integers.

Fix k and let $w(s) = \sin(k\pi s)$ in (5.14). By explicit computations, we have that (5.15) becomes

$$\dot{\lambda}_{n,m}(0) = -\Big(\frac{m\pi}{4l}\Big)^2 \int_0^1 \sin^2(n\pi s)\sin(k\pi s)\, ds.$$

Thus,

$$\dot{\lambda}_{n,m}(0) = \begin{cases} 0 & k \text{ even}, \\ \dfrac{(nm)^2\pi}{4kl^2(k^2-4n^2)} & k \text{ odd}. \end{cases}$$

Therefore, if k is odd,

$$\lambda_{n,m}(t) - \lambda_{n,m}(0) = t\frac{(nm)^2\pi}{4kl^2(k^2-4n^2)} + O(t^2), \tag{5.16}$$

and so we can recover a first-order approximation of t from the knowledge of a single arbitrary eigenvalue shift. To find an approximation of t when k is even, we would need higher-order terms.

Suppose now that we want to determine the shape of the internal cavity inside a hollow cylinder, knowing that it is a small perturbation of a concentric cylinder. For simplicity, we reduce our analysis to a two dimensional section, but the same technique used for this case can be adapted to the higher dimensions.

Example 5.9 (Internal deformation of an annulus). Let Ω be an annulus of external radius 2 and internal radius 1. Let Γ^e, Γ^i indicate respectively the circle of radius 2 and the circle of radius 1. By separation of variables, it can be shown that the Dirichlet eigenfunctions of Ω associated to an eigenvalue $\lambda_{n,k}$, with $n \in \mathbb{N}$ and $k \in \mathbb{Z}^+$, can be written in polar coordinates as

$$u_{n,k}(r, \mathfrak{t}) = R_{n,k}(r)\cos(n\mathfrak{t}), \tag{5.17}$$

$$v_{n,k}(r, \mathfrak{t}) = R_{n,k}(r)\sin(n\mathfrak{t}), \tag{5.18}$$

where

$$R_{n,k}(r) = \alpha_n\big(J_n(\sqrt{\lambda_{n,k}}r) + c_{n,k}Y_n(\sqrt{\lambda_{n,k}}r)\big), \tag{5.19}$$

and the constants $\lambda_{n,k}$ and $c_{n,k}$ are determined by the boundary conditions on Γ^e and Γ^i, and α_n is a normalization constant so that the eigenfunctions have L^2-norm equal to 1.

Let Ω_ε be given by a constant speed deformation of the internal circle Γ^i with shape $w \in \mathrm{C}^2(\Gamma^i)$; that is, $\partial\Omega_\varepsilon$ is given by two disconnected sets $\Gamma^e_\varepsilon, \Gamma^i_\varepsilon$ such that $\Gamma^e_\varepsilon = \Gamma^e$ and $\Gamma^i_\varepsilon = \Gamma^i + \varepsilon w(\Gamma^i)\nu$. The geometry of the problem allows us to expand w in a Fourier series

$$w(\mathsf{t}) = \sum_{j=1}^{\infty} b_j \sin(j\mathsf{t}), \tag{5.20}$$

with $b_j \geq 0$. We can also explicitly compute that the $O(\varepsilon^2)$ approximation of $\lambda^1_{\varepsilon,n,k} - \lambda_{n,k}$ is given by

$$\begin{aligned}
&-\varepsilon \min_{A,B:A^2+B^2=1} \int_{\Gamma^i} \big(\partial(Au_{n,k} + Bv_{n,k})/\partial\nu\big)^2 w && (5.21)\\
&= \varepsilon R'_{n,k}(1) \min_{\varphi\in[0,2\pi]} \int_0^{2\pi} \frac{1+\sin(2\varphi)\sin(2n\mathsf{t}) + \cos(2\varphi)\cos(2n\mathsf{t})}{2} w(\mathsf{t})\, d\mathsf{t} && (5.22)\\
&= \frac{\varepsilon\pi}{2} R'_{n,k}(1) \min_{\varphi\in[0,2\pi]} b_{2n}\sin(2\varphi). && (5.23)
\end{aligned}$$

Therefore

$$\begin{aligned}
\lambda^1_{\varepsilon,n,k} - \lambda_{n,k} &= -\frac{\varepsilon\pi}{2} R'_{n,k}(1)|b_{2n}| + O(\varepsilon^2), && (5.24)\\
\lambda^2_{\varepsilon,n,k} - \lambda_{n,k} &= O(\varepsilon^2). && (5.25)
\end{aligned}$$

Thus, we can recover the $2n$-th coefficient of the Fourier series of w directly from the shift of the smallest eigenvalue perturbed from $\lambda_{n,k}$, for an arbitrary choice of k.

Chapter 6

Perturbation of scattering resonances - transverse magnetic polarization case

The influence of a small particle on a cavity mode plays an important role in fields such as optical sensing, cavity quantum electrodynamics, and cavity optomechanics [53, 92, 82]. In this chapter, we consider the transverse magnetic polarization case and provide a formal derivation of the perturbations of scattering resonances of an open cavity due to a small-volume particle without neglecting the radiation effect. Note that the radiation effect has been omitted in the physics literature (see, for instance, [45]). Indeed, the Bethe-Schwinger closed cavity perturbation formula [23, 31] has been widely employed for radiating cavities. The small-volume asymptotic formula in this chapter generalizes to the open cavity case those derived in [14, 16, 78, 23]. It is valid for arbitrary-shaped particles. It shows that the perturbations of the scattering resonances can be expressed in terms of the polarization tensor of the small particle. Two cases are considered: the one-dimensional case and the multi-dimensional case. Its applicability to the perturbations of whispering-gallery modes by external arbitrary-shaped particles is also discussed. Finally, we characterize the effect that a plasmonic nanoparticle, of arbitrary geometry and which is bound to the surface of the cavity, has on the whispering-gallery modes of the cavity. Since the shift of the scattering frequencies is proportional to the polarization of the plasmonic nanoparticles [8, 17, 18, 21], which blows-up at the plasmonic resonances, the effect of a plasmonic particle on the cavity modes can be significant.

For the analysis of the transverse electric case we refer to Chapter 7. Note that in the one-dimensional case, the scattering resonances are simple while in the multi-dimensional case, they can be degenerate or even exceptional. The analysis of exceptional points is a challenging problem, and the situation is much simpler in the transverse electric case than in the transverse magnetic one. The reader is also referred to [54, 55, 63] for small amplitude sensitivity analyses of the scattering resonances. Numerical computation of resonances has been addressed, for instance, in [50, 64, 70, 71, 85, 100].

The chapter is organized as follows. In Section 6.1, using the method of matched asymptotic expansions, we derive the leading-order term in the shifts of scattering resonances of a one-dimensional open cavity and characterize the effect of radiation. Section 6.2 generalizes the method to the multi-dimensional case. In Section 6.3, we consider the perturbation of whispering-gallery modes by small particles. The formula obtained for the shifting of the frequencies shows a strong enhancement in the frequency shift in the case of plasmonic particles, which allows for their recognition in spite of their small size. The splitting of scattering frequencies of the open cavity of multiplicity greater than one due to small particles is also discussed. In Section 6.4, we present some numerical examples to illustrate the accuracy of the formulas derived in this chapter and their use in the sensing of small particles. The chapter ends with some concluding remarks.

6.1 One dimensional case

We first consider a one dimensional cavity. We let the magnetic permeability μ_δ be μ_m in $(a,b) \setminus (-\delta/2, \delta/2)$ and μ_c in $(-\delta/2, \delta/2)$ and the electric permittivity ε_δ be ε_m in $(a,b) \setminus (-\delta/2, \delta/2)$ and ε_c in $(-\delta/2, \delta/2)$. Here, $0 < \delta < 1/2$ and $\mu_m, \mu_c, \varepsilon_m$, and ε_c are positive constants.

Let ω_0 be a scattering resonance of the unperturbed cavity and let u_0 denote the corresponding eigenfunction, that is,

$$\begin{cases} \partial_x\left((1/\varepsilon_m)\partial_x u_0\right) + \omega_0^2 \mu_m u_0 = 0 & \text{in } (a,b), \\ (1/\varepsilon_m)\partial_x u_0 + \mathrm{i}\omega_0 u_0 = 0 & \text{at } a, \\ (1/\varepsilon_m)\partial_x u_0 - \mathrm{i}\omega_0 u_0 = 0 & \text{at } b, \\ \int_a^b |u_0|^2 \, dx = 1. \end{cases}$$

We now consider the perturbed problem: for δ small, we seek a solution u_δ, for which $\omega_\delta \to \omega_0$ as $\delta \to 0$ of the following equation:

$$\begin{cases} \partial_x\left((1/\varepsilon_\delta)\partial_x u_\delta\right) + \omega_\delta^2 \mu_\delta u_\delta = 0 & \text{in } (a,b), \\ (1/\varepsilon_m)\partial_x u_\delta + \mathrm{i}\omega_\delta u_\delta = 0 & \text{at } a, \\ (1/\varepsilon_m)\partial_x u_\delta - \mathrm{i}\omega_\delta u_\delta = 0 & \text{at } b, \\ \int_a^b |u_\delta|^2 \, dx = 1. \end{cases} \tag{6.1}$$

Remark 6.1. The above one-dimensional scattering resonance problems govern scattering resonances of slab-type structures. They are a consequence of Maxwell's equations, under the assumption of time-harmonic solutions. They correspond to the transverse magnetic polarization; see [55]. The scattering resonances ω_0 and ω_δ lie in the lower-half of the complex plane. The eigenfunctions u_0 and u_δ satisfy the outgoing radiation conditions at a and b and, consequently, grow exponentially at large distances from the cavity. To give a physical interpretation of scattering resonances see, for instance, [50, 55].

Proposition 6.2. *Assuming that*

$$\omega_\delta = \omega_0 + \delta\omega_1 + \dots,$$

we have

$$\omega_1 = \frac{\alpha(\partial_x u_0(0))^2 + \omega_0^2 \varepsilon_m(\mu_c - \mu_m)(u_0(0))^2}{2\omega_0\mu_m\varepsilon_m + \mathrm{i}\varepsilon_m((u_0(a))^2 + (u_0(b))^2)}, \tag{6.2}$$

where the polarization α is defined by

$$\alpha = 1 - \frac{\varepsilon_c}{\varepsilon_m}. \tag{6.3}$$

Proof. Using the method of matched asymptotic expansions for δ small, see [16], we construct asymptotic expansions of ω_δ and u_δ.

To reveal the nature of the perturbations in u_δ, we introduce the local variable $\xi = x/\delta$ and set $e_\delta(\xi) = u_\delta(x)$. We expect that $u_\delta(x)$ will differ appreciably from

$u_0(x)$ for x near 0, but it will differ little from $u_0(x)$ for x far from 0. Therefore, in the spirit of matched asymptotic expansions, we shall represent u_δ by two different expansions, an inner expansion for x near 0, and an outer expansion for x far from 0. We write the outer and inner expansions:

$$u_\delta(x) = u_0(x) + \delta u_1(x) + \dots \quad \text{for } |x| \gg \delta,$$

and

$$u_\delta(x) = e_0(\xi) + \delta e_1(\xi) + \dots \quad \text{for } |x| = O(\delta).$$

The asymptotic expansion of ω_δ must begin with ω_0, so we write

$$\omega_\delta = \omega_0 + \delta\omega_1 + \dots.$$

In order to determine the functions $u_i(x)$ and $e_i(\xi)$, we have to equate the inner and the outer expansions in some "overlap" domain within which the stretched variable ξ is large and x is small. In this domain the matching conditions are:

$$u_0(x) + \delta u_1(x) + \dots \sim e_0(\xi) + \delta e_1(\xi) + \dots.$$

Now, if we substitute the inner expansion into (6.1) and formally set to zero the coefficients of δ^{-2} and δ^{-1}, then we obtain

$$\partial_\xi((1/\tilde{\varepsilon})\partial_\xi e_i) = 0, \quad \text{for } i = 0, 1,$$

where the stretched coefficient $\tilde{\varepsilon}$ is equal to ε_c in $(-1/2, 1/2)$ and to ε_m in $(-\infty, -1/2)\cup(1/2, +\infty)$. From the first matching condition, it follows that $e_0(\xi) = u_0(0)$ for all ξ. Similarly, we have

$$e_1(\xi) \sim \xi\partial_x u_0(0) \quad \text{as } |\xi| \to +\infty. \tag{6.4}$$

Let $v^{(1)}(\xi)$ be such that

$$\begin{cases} \partial_\xi((1/\tilde{\varepsilon}(\xi))\partial_\xi v^{(1)}(\xi)) = 0, \\ v^{(1)}(\xi) \sim \xi \quad \text{as } |\xi| \to +\infty. \end{cases}$$

Although $v^{(1)}$ can be trivially rewritten as a piecewise affine function, let us take an approach which generalizes easily to the multi-dimensional case. Let $\gamma = (\varepsilon_m/\varepsilon_c) - 1$. By how $v^{(1)}$ is defined, we have

$$v^{(1)}(\xi) = \xi - \gamma\partial_\xi v^{(1)}(-1/2)|_+\Gamma_0(\xi + 1/2) + \gamma\partial_\xi v^{(1)}(1/2)|_-\Gamma_0(\xi - 1/2),$$

where the subscripts + and − indicate respectively the limits at 1/2 from the left and from the right. Moreover,

$$\int_{-1/2}^{1/2} \partial_\xi^2 v^{(1)}\, d\xi = 0,$$

yields

$$\partial_\xi v^{(1)}(-1/2)|_+ = \partial_\xi v^{(1)}(1/2)|_-.$$

Hence,

$$v^{(1)}(\xi) = \xi + \gamma \partial_\xi v^{(1)}(1/2)|_- G(\xi + 1/2) - \gamma \partial_\xi v^{(1)}(1/2)|_- G(\xi - 1/2).$$

On the other hand,

$$G(\xi \pm 1/2) \sim |\xi| \pm \xi/(2|\xi|) + \dots \quad \text{as } |\xi| \to +\infty.$$

Therefore,

$$v^{(1)}(\xi) \sim \xi - ((\varepsilon_m/\varepsilon_c) - 1)\partial_\xi v^{(1)}(1/2)|_-\ \xi/|\xi| + \dots.$$

From [16, (4.11)], we have that $e_1(\xi) = (\partial_x u_0)(0)v^{(1)}(\xi)$. By matching the first-order terms in the inner and outer expansion we obtain $u_1(x) \sim e_1(\xi) - \xi(\partial_x u_0)(0)$. Then, the second matching condition (6.4) yields

$$u_1(x) \sim -\gamma(\partial_x u_0(0))(\partial_\xi v^{(1)}(1/2)|_-)(\xi/|\xi|) \quad \text{for } x \text{ near } 0.$$

Assume first that $\mu_m = \mu_c$. To find the first correction ω_1, we multiply

$$\partial_x((1/\varepsilon_m)\partial_x u_1) + \omega_0^2 \mu_m u_1 = -2\omega_1\omega_0\mu_m u_0$$

by u_0 and integrate over $(a, -\rho/2)$ and $(\rho/2, b)$ for $\rho \geq \delta$. Upon using the radiation conditions, integration by parts, and the asymptotics of u_1 previously derived, we obtain that as ρ and δ go to zero,

$$\mathrm{i}\omega_1((u_0(a))^2 + (u_0(b))^2) - \frac{1}{\varepsilon_m}\alpha(\partial_x u_0(0))^2 = -2\omega_1\omega_0\mu_m,$$

where the polarization α is given by

$$\alpha = \gamma\partial_\xi v^{(1)}(1/2)|_- = 1 - \frac{\varepsilon_c}{\varepsilon_m}. \tag{6.5}$$

Therefore, we arrive at

$$\omega_1 = \frac{\alpha(\partial_x u_0(0))^2}{2\omega_0\mu_m\varepsilon_m + \mathrm{i}\varepsilon_m((u_0(a))^2 + (u_0(b))^2)}. \tag{6.6}$$

The term $\mathrm{i}\varepsilon_m((u_0(a))^2 + (u_0(b))^2)$ accounts for the effect of radiation on the shift of the scattering resonance ω_0.

Now, if $\mu_c \neq \mu_m$, we need to compute the second-order corrector e_2. We have

$$\partial_\xi((1/\tilde{\varepsilon})\partial_\xi e_2) + \omega_0^2 \tilde{\mu} e_0 = 0,$$

and

$$e_2(\xi) \sim \xi^2 \partial_x^2 u_0(0)/2 \quad \text{as } |\xi| \to +\infty.$$

here, the stretched coefficient $\tilde{\mu}$ is equal to μ_c in $(-1/2, 1/2)$ and to μ_m in $(-\infty, -1/2) \cup (1/2, +\infty)$.

From the equation satisfied by u_0, we obtain

$$\partial_x^2 u_0(0) = -\omega_0^2 \mu_m \varepsilon_m u_0(0).$$

Recall that $e_0(\xi) = u_0(0)$ and let $v^{(2)}$ be such that

$$\begin{cases} \partial_\xi((1/\tilde{\varepsilon}(\xi))\partial_\xi v^{(2)}(\xi)) = (1/(\varepsilon_m \mu_m))\tilde{\mu}(\xi), \\ v^{(2)}(\xi) \sim \xi^2/2 \quad \text{as } |\xi| \to +\infty. \end{cases}$$

It is easy to see that $\partial_\xi((1/\tilde{\varepsilon}(\xi))\partial_\xi(v^{(2)}(\xi) - \xi^2/2))$ is $(1/\varepsilon_m)((\mu_c/\mu_m) - 1)$ for $\xi \in (-1/2, 1/2)$ and is 0 for $|\xi| > 1/2$. Therefore,

$$v^{(2)}(\xi) - \xi^2/2 \sim ((\mu_c/\mu_m) - 1)|\xi| \quad \text{as } |\xi| \to +\infty.$$

Then, by matching the singularities in the inner and outer expansion as in [16, Section 4.1], we obtain

$$u_1(x) \sim \partial_x u_0(0)(\xi - ((\varepsilon_m/\varepsilon_c) - 1)\partial_\xi v^{(1)}(1/2)\xi/|\xi| + \ldots) + \partial_x^2 u_0(0)((\mu_c/\mu_m) - 1)|\xi| + \ldots,$$

and so, proceeding as before,

$$\begin{aligned} \mathrm{i}\omega_1((u_0(a))^2 + (u_0(b))^2) - \frac{1}{\varepsilon_m}\alpha(\partial_x u_0(0))^2 + \frac{1}{\varepsilon_m}\partial_x^2 u_0(0)((\mu_c/\mu_m) - 1)u_0(0) \\ = -2\omega_1\omega_0\mu_m, \end{aligned}$$

which yields the result. □

6.2 Multi-dimensional case

In this section, we generalize (6.2) to the multi-dimensional case. In dimension two, the obtained formula corresponds, as in the one-dimensional case, to an open cavity with the transverse magnetic polarization [63]. We use the same notation as in Section 6.2.

Let Ω be a bounded domain in $\mathbb{R}^d$ for $d = 2, 3$, with smooth boundary $\partial\Omega$. We assume ω_0 is a simple scattering resonance of the unperturbed open cavity, that is there exists a unique non trivial solution u_0 to

$$\begin{cases} \nabla \cdot ((1/\varepsilon)\nabla u) + \omega_0^2 \mu u = 0 \quad \text{in } \mathbb{R}^d, \\ \displaystyle\int_\Omega |u|^2 \, dx = 1, \\ u \text{ satisfies the Sommerfeld radiation condition,} \end{cases} \tag{6.7}$$

where $\mu = 1+(\mu_m-1)\chi_\Omega$ and $\varepsilon = 1+(\varepsilon_m-1)\chi_\Omega$. Here, χ_Ω denotes the characteristic function of the domain Ω.

For simplicity, we assume that Ω is the ball of radius R centered at the origin, and introduce the capacity operator T_ω, which is given by [20]

$$T_\omega : \phi = \begin{cases} \displaystyle\sum_{m\in\mathbb{Z}} \phi_m e^{im\theta} & \text{if } d = 2, \\ \displaystyle\sum_{m=0}^{+\infty} \sum_{l=-m}^{m} \phi_m^l Y_m^l & \text{if } d = 3, \end{cases} \mapsto \begin{cases} \displaystyle\sum_{m\in\mathbb{Z}} z_m(\omega, R) \phi_m e^{im\theta} & \text{if } d = 2, \\ \displaystyle\sum_{m=0}^{+\infty} z_m(\omega, R) \sum_{l=-m}^{m} \phi_m^l Y_m^l & \text{if } d = 3, \end{cases}$$

where

$$z_m(\omega, R) = \begin{cases} \dfrac{\omega (H_m^{(1)})'(\omega R)}{H_m^{(1)}(\omega R)} & \text{if } d = 2, \\ \dfrac{\omega (h_m^{(1)})'(\omega R)}{h_m^{(1)}(\omega R)} & \text{if } d = 3. \end{cases}$$

Here, θ is the angular variable, Y_m^l is a spherical harmonic, and $H_m^{(1)}$ (respectively, $h_m^{(1)}$) is the Hankel function of integer order (respectively, half-integer order). This explicit version of the capacity operator will be used in Section 6.4 to test the validity of our formula. Then, (6.7) is equivalent to

$$\begin{cases} (1/\varepsilon_m)\Delta u_0 + \omega_0^2 \mu u_0 = 0 \quad \text{in } \Omega, \\ (1/\varepsilon_m)\dfrac{\partial u_0}{\partial \nu} = T_{\omega_0}[u_0] \quad \text{on } \partial\Omega, \\ \int_\Omega |u_0|^2 = 1, \end{cases} \tag{6.8}$$

where ν denotes the normal to $\partial\Omega$. As in the one-dimensional case, the scattering resonances lie in the lower-half of the complex plane and the associated eigenfunctions grow exponentially at large distances from the cavity since they satisfy the outgoing radiation condition. We also remark that from Green's identity we have

$$\int_{\partial\Omega} T_\omega[f] g \, d\sigma = \int_{\partial\Omega} f T_\omega[g] \, d\sigma \quad \text{for all } f, g \in \mathrm{H}^{1/2}(\partial\Omega), \tag{6.9}$$

for $d = 2, 3$.

Let $D \Subset \Omega$ be a small particle of the form $D = z+\delta B$, where δ is its characteristic size, z its location, and B is a smooth bounded domain containing the origin. Denote respectively by ε_c and μ_c the electric permittivity and the magnetic permeability of the particle D. The eigenvalue problem is to find ω_δ such that there is a non-trivial couple $(\omega_\delta, u_\delta)$ satisfying

$$\begin{cases} (1/\varepsilon_m)\Delta u_\delta + \omega_\delta^2 \mu_m u_\delta = 0 & \text{in } \Omega \setminus \bar{D}, \\ (1/\varepsilon_c)\Delta u_\delta + \omega_\delta^2 \mu_c u_\delta = 0 & \text{in } D, \\ (1/\varepsilon_m)\dfrac{\partial u_\delta}{\partial \nu}\Big|_+ = (1/\varepsilon_c)\dfrac{\partial u_\delta}{\partial \nu}\Big|_- & \text{on } \partial D, \\ (1/\varepsilon_m)\dfrac{\partial u_\delta}{\partial \nu} = T_{\omega_\delta}[u_\delta] & \text{on } \partial\Omega, \end{cases} \tag{6.10}$$

where the subscripts $+$ and $-$ indicate the limits from outside and inside D, respectively.

Proposition 6.3. *Assuming $\omega_\delta = \omega_0 + \delta^d \omega_1 + \dots$, we have*

$$\omega_1 = \frac{M(\varepsilon_m/\varepsilon_c, B)\nabla u_0(z) \cdot \nabla u_0(z) + \omega_0^2 |B| \varepsilon_m (\mu_c - \mu_m)(u_0(z))^2}{2\omega_0 \mu_m \varepsilon_m \int_\Omega u_0^2 \, dx + \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0] u_0 \, d\sigma}, \tag{6.11}$$

where M is the polarization tensor defined in (1.11).

Proof. Assume, for now, that $\mu_c = \mu_m$. Let $\lambda_0 = \omega_0^2, \lambda_\delta = \omega_\delta^2$. We expand

$$\omega_\delta = \omega_0 + \delta^d \omega_1 + \dots \quad \text{and} \quad \lambda_\delta = \lambda_0 + \delta^d \lambda_1 + \dots .$$

Let the outer expansion of u_δ be

$$u_\delta(y) = u_0(y) + \delta^d u_1(y) + \dots ,$$

and the inner one, $e_\delta(\xi) = u_\delta((x-z)/\delta)$, be

$$e_\delta(\xi) = e_0(\xi) + \delta e_1(\xi) + \dots .$$

Therefore, formally we have

$$T_{\omega_\delta} \simeq T_{\omega_0 + \delta^d \omega_1} \simeq T_{\omega_0} + \delta^d \omega_1 \partial_\omega T_\omega|_{\omega_0} + \dots .$$

Moreover, we obtain

$$\begin{cases} ((1/\varepsilon_m)\Delta + \lambda_0 \mu_m) u_1(y) = -\lambda_1 \mu_m u_0(y) & \text{for } |y-z| \gg O(\delta), \\ (1/\varepsilon_m)\dfrac{\partial u_1}{\partial \nu} = T_{\omega_0}[u_1] + \omega_1 \partial_\omega T_\omega|_{\omega=\omega_0}[u_0] & \text{on } \partial\Omega, \end{cases} \tag{6.12}$$

and, by setting to zero the coefficients of $1/\delta^2$ and $1/\delta$ in e_δ in (6.10),

$$\begin{cases} \Delta_\xi e_j = 0 & \text{in } \mathbb{R}^d \setminus (\partial B), \\ \dfrac{\partial e_j}{\partial \nu}|_+ = (\varepsilon_m/\varepsilon_c)\dfrac{\partial e_j}{\partial \nu}|_- & \text{on } \partial B, \end{cases}$$

for $j = 0, 1$. Imposing the matching conditions

$$u_0(y) + \delta^d u_1(y) + \cdots \sim e_0(\xi) + \delta e_1(\xi) + \ldots \quad \text{as } |\xi| \to +\infty,$$

and $y \to z$, we arrive at $e_0(\xi) \to u_0(z)$ and $e_1(\xi) \sim \nabla u_0(z) \cdot \xi$. So, we have $e_0(\xi) = u_0(z)$ for every ξ and $e_1(\xi) = \nabla u_0(z) \cdot v^{(1)}(\xi)$, where $v^{(1)}$ is such that (see [16, (4.11)])

$$\begin{cases} \Delta_\xi v^{(1)} = 0 & \text{in } \mathbb{R}^d \setminus (\partial B), \\ \dfrac{\partial v^{(1)}}{\partial \nu}|_+ = (\varepsilon_m/\varepsilon_c)\dfrac{\partial v^{(1)}}{\partial \nu}|_- & \text{on } \partial B, \\ v^{(1)}(\xi) \sim \xi & \text{as } |\xi| \to +\infty. \end{cases} \tag{6.13}$$

Let $M(\varepsilon_m/\varepsilon_c, B)$ be the polarization tensor associated with the domain B and the contrast $\varepsilon_m/\varepsilon_c$. Then, by the same arguments as in [16, Section 4.1], it follows that

$$u_1(y) \sim -M(\varepsilon_m/\varepsilon_c, B)\nabla\Gamma(y-z)\cdot\nabla u_0(z) \quad \text{as } y \to z. \tag{6.14}$$

Multiplying (6.12) by u_0 and integrating by parts over $\Omega \setminus \bar{B}_\delta$, we obtain from (6.9), the identity $(-1/\varepsilon_m)\Delta u_0 = \lambda_0 \mu_m u_0$, that

$$\begin{aligned} -\lambda_1\mu_m \int_{\Omega\setminus B_\delta} (u_0)^2\, dx \;\; = \;\; & \underbrace{\int_{\partial\Omega} \big(T_{\omega_0}[u_1]u_0 - T_{\omega_0}[u_0]u_1\big)\, d\sigma}_{=0} + \omega_1 \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0\, d\sigma \\ & + \frac{1}{\varepsilon_m}\int_{\partial B_\delta} (u_0 \frac{\partial u_1}{\partial \nu} - u_1 \frac{\partial u_0}{\partial \nu})\, d\sigma. \end{aligned}$$

From (6.14), we have

$$\int_{\partial B_\delta} (u_0 \frac{\partial u_1}{\partial \nu} - u_1 \frac{\partial u_0}{\partial \nu})\, d\sigma \xrightarrow[\delta\to 0]{} -M(\varepsilon_m/\varepsilon_c, B)\nabla u_0(z)\cdot\nabla u_0(z).$$

Therefore, since $\lambda_1 = 2\omega_0\omega_1$,

$$-\lambda_1\mu_m\varepsilon_m \int_\Omega u_0^2\, dx - \frac{\lambda_1}{2\omega_0}\int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0\, d\sigma = -M(\varepsilon_m/\varepsilon_c, B)\nabla u_0(z)\cdot\nabla u_0(z),$$

and finally, we arrive at

$$\lambda_1 = \frac{M(\varepsilon_m/\varepsilon_c, B)\nabla u_0(z)\cdot\nabla u_0(z)}{\varepsilon_m\mu_m \int_\Omega u_0^2\, dx + (1/(2\omega_0))\int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0\, d\sigma}, \tag{6.15}$$

or equivalently,

$$\omega_1 = \frac{M(\varepsilon_m/\varepsilon_c, B)\nabla u_0(z) \cdot \nabla u_0(z)}{2\omega_0\mu_m\varepsilon_m \int_\Omega u_0^2\, dx + \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0\, d\sigma}. \tag{6.16}$$

If one relaxes the assumption $\mu_c = \mu_m$, one can generalize formula (6.16) by computing, as in [16] and in Section 6.1, the second-order corrector e_2. We then get the desired result. $\square$

The expression derived in Proposition 6.3 tells us that in the multi-dimensional case, the effect of radiation on the shift of the scattering resonance ω_0 is given by $\int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0\, d\sigma$. Note also that (6.16) reduces to (6.6) in the one-dimensional case. In fact, the polarization tensor M reduces to α defined by (6.5) and the operator T_ω corresponds to the multiplication by $-\mathrm{i}\omega\varepsilon_m$ at a and $+\mathrm{i}\omega\varepsilon_m$ at b.

6.3 Perturbation of whispering-gallery modes by an external particle

Whispering-gallery modes are modes which are confined near the boundary of the cavity. Their existence for spherical resonators can be proved analytically or by a boundary layer approach based on WKB (high frequency) asymptotics [82, 68, 72, 75, 45, 84, 1]. Whispering-gallery modes can be exploited to probe the local surroundings of the resonator [65, 66, 83]. Biosensors based on the shift of whispering-gallery modes in open cavities by small particles have been also described by use of Bethe-Schwinger type formulas, where the effect of radiation is neglected [26, 45, 98, 99]. In this section, we provide a generalization of the formula derived in the previous section and discuss its validity for whispering-gallery modes.

Assume that ω_0 is a whispering-gallery mode of the open cavity Ω. Let Ω_ρ be a small neighborhood of Ω. Suppose that the particle D is in $\Omega_\rho \setminus \overline{\Omega}$. If the characteristic size δ of D is much smaller than ρ, which is in turn much smaller than $2\pi/(\sqrt{\varepsilon_m\mu_m}\omega_0)$, then by the same arguments as those in the previous section, the leading-order term in the shift of the resonant frequency ω_0 is given by

$$\omega_1 \simeq \frac{M(1/\varepsilon_c, B)\nabla v_0(z) \cdot \nabla v_0(z) + \omega_0^2|B|(\mu_c - 1)(v_0(z))^2}{2\omega_0\mu_m\varepsilon_m \int_\Omega u_0^2\, dx + \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0\, d\sigma}.$$

Here, the polarization tensor $M(\varepsilon_m/\varepsilon_c, B)$ in (6.15) is replaced by $M(1/\varepsilon_c, B)$ since

ε in the medium surrounding the particle is equal to 1 and v_0 is defined in $\mathbb{R}^d$ by

$$v_0(x) = -\omega_0^2(\mu_m - 1)\int_\Omega \Gamma(x-y;\omega_0)u_0(y)\,dy + (\frac{1}{\varepsilon_m} - 1)\int_\Omega \nabla_y \Gamma(x-y;\omega_0)\cdot\nabla u_0(y)\,dy, \tag{6.17}$$

where $\Gamma(\cdot;\omega_0)$ is the fundamental solution of $\Delta + \omega_0^2$, which satisfies the outgoing radiation condition. We remark that $v_0 = u_0$ in Ω. Moreover, the assumption that ω_0 is a whispering-gallery mode is needed in order to have the gradient of v_0 at the location of the particle to have a significant magnitude.

Now, assume that the particle D is plasmonic, i.e., ε_c depends on the frequency ω and can take negative values. In this case, there is a discrete set of frequencies, called plasmonic resonant frequencies, such that at these frequencies problem (6.13) is nearly singular, and therefore the polarization tensor associated with the particle D blows up at those frequencies, see [8, 18, 21]. Assume that the plasmonic particle is coupled to the cavity, i.e., there is a whispering-gallery cavity mode ω_0 such that $\Re\omega_0$ is a plasmonic resonance of the particle.

Then when the particle D is illuminated at the frequency $\Re\omega_0$, its effect on the cavity mode ω_0 is given by

$$\omega_1 \simeq \frac{M((1/\varepsilon_c)(\Re\omega_0), B)\nabla v_0(z)\cdot\nabla v_0(z) + \omega_0^2|B|(\mu_c - 1)(v_0(z))^2}{2\omega_0\mu_m\varepsilon_m\int_\Omega u_0^2\,dx + \int_{\partial\Omega}\partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0\,d\sigma}, \tag{6.18}$$

where v_0 is defined by (6.17). Thus, despite their small size, plasmonic particles can significantly change the cavity modes when their plasmonic resonances are close to the cavity modes.

Finally, let us briefly consider the case when there are multiple linear independent solutions to (6.7). This situation has been studied in Chapter 4 for closed cavities, under the much simpler setting of a self-adjoint operator. Although the extension of the formulae derived in this simpler setting to open resonators would require a finer analysis, we believe that similar expressions still hold. In fact, in the next section we provide numerical evidence to the fact that, if there are two orthogonal solutions u_1, u_2 to (6.7), then the largest and smallest resonance perturbations are indeed proportional respectively to the largest and smallest eigenvalues of the matrix

$$\Big(M((1/\varepsilon_c)(\Re\omega_0), B)\nabla u_i(z)\cdot\nabla u_j(z)\Big)_{i,j\in\{1,2\}}. \tag{6.19}$$

6.4 Numerical illustrations

In two dimensions, when the cavity and the small-volume particle are disks we can use the multipole expansion method to efficiently compute the perturbations of the whispering-gallery modes [74]. Our approach is as follows. We first use a projective eigensolver [29] to obtain a coarse estimate of the locations of the resonances of a two disk system. We then focus on the particular resonances in this set that correspond to the whispering-gallery modes of the open cavity and obtain a refined estimate of their locations using the multipole method.

Throughout this section, Ω is a disk of radius 1 centered at the origin and ω_0 is the frequency of a whispering-gallery mode. Let D be a disk of radius δ centered at $(1 + 2\delta, 0)$. Suppose that $\varepsilon_m = \varepsilon_c = 1/5$. The behavior of $\omega_{\delta,1}, \omega_{\delta,2}$ as $\delta \to 0$ is plotted in Figure 6.1. The characterization of multiple resonances given in (6.19) matches the first resonance shift, as can be seen in Figure 6.2. On the other hand, we can easily reconstruct δ from a single scattering resonance shift.

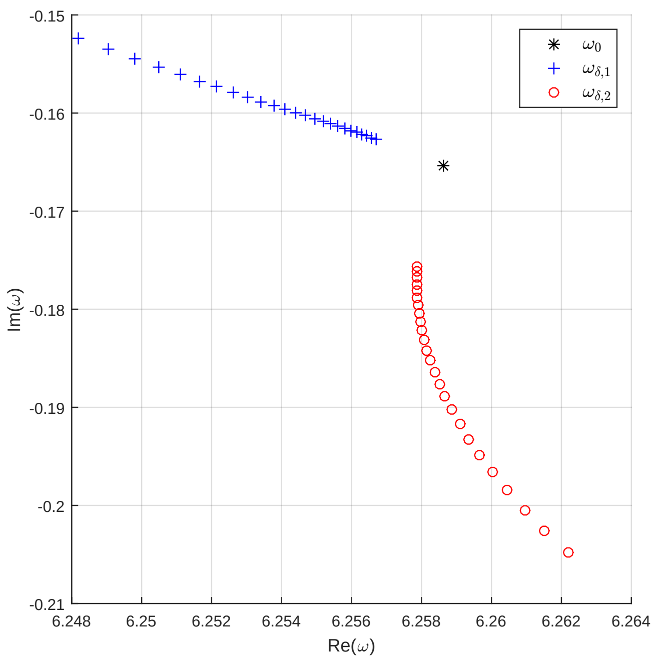


Figure 6.1: As the size of the small disk $\delta \to 0$, the perturbed whispering-gallery modes $\omega_{\delta,1}$ and $\omega_{\delta,2}$ converge towards the unperturbed mode ω_0.

Next, consider a disk D_δ of radius $\delta = 0.1$ centered at $(z, 0)$. A plot of $|\omega_{\delta,j}^2 - \omega_0^2|$ as z varies between 1.2 and 6 is presented in Figure 6.3. We remark that the again

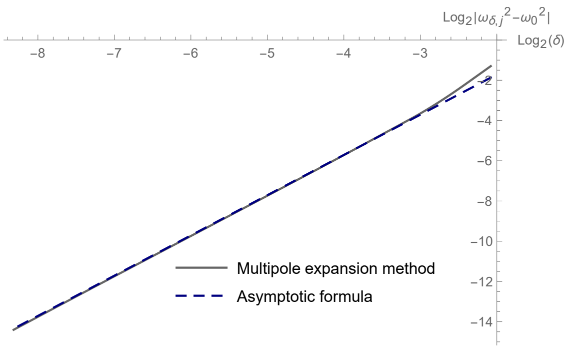


Figure 6.2: Comparison between the asymptotic formula for the perturbation $|\omega_{\delta,1}^2 - \omega_0^2|$ of the whispering-gallery mode and the perturbation computed numerically as the size of the small disk $\delta \to 0$.

characterization of multiple resonances given in (6.19) matches closely the numerical experiments.

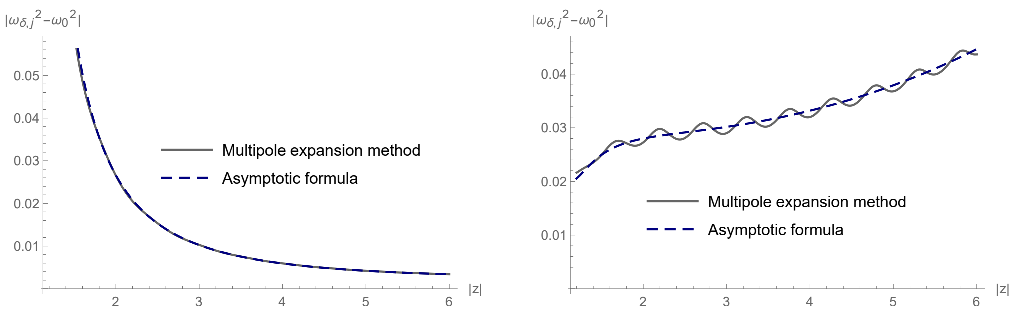


Figure 6.3: Comparison between the asymptotic formula for the perturbation $|\omega_{\delta,j}^2 - \omega_0^2|$ of the whispering-gallery mode and the perturbation computed numerically as the position of the inclusion $(z, 0)$ varies. The plot on the left corresponds to the perturbed resonance $\omega_{\delta,1}$ and the plot on the right corresponds to the perturbed resonance $\omega_{\delta,2}$.

We highlight now the case of plasmonic particles. In this case we have a strong enhancement in the frequency shift, which allows for the recognition of much smaller particles. Consider a disk D of radius 0.1 centered at $(1.2, 0)$. Suppose $\varepsilon_m = 1/5$. A plot of numerical experiments for the shift $|\omega_{\delta,1}^2 - {\omega_0}^2|$ as $1/\varepsilon_c$ varies is presented in Figure 6.4. Notice the high peak in the perturbation as ε_c approaches the value -1.

Finally, let us remark that our formulae also allow quick estimates of the polarization tensor of the small particle. Thus the orientation of the perturbing particle can be inferred, which affords the possibility of orientational binding studies in biosensing. We also believe that, based on [23, 13], the derived formulae can be generalized to open electromagnetic and elastic cavities.

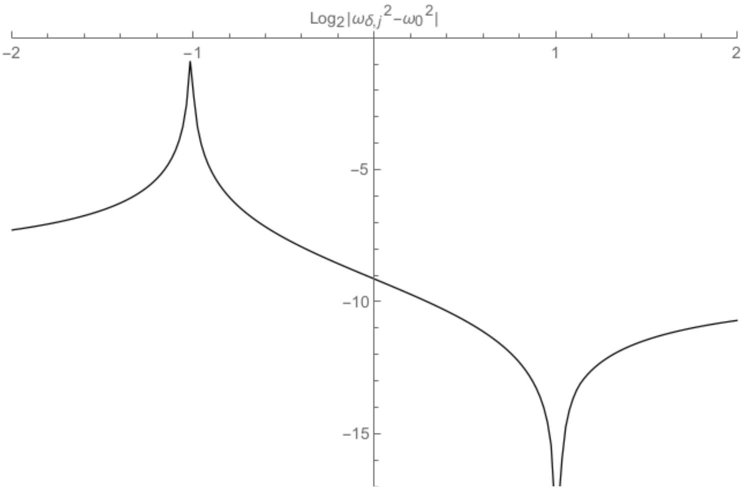


Figure 6.4: Resonance perturbation $|\omega_{\delta,1}^2 - \omega_0^2|$ as a function of $1/\varepsilon_c$, here allowed to also take negative values.

Chapter 7

Perturbation of scattering resonances - transverse electric polarization case

In this chapter we consider dielectric radiating open cavities [27, 34, 94] and rigorously obtain asymptotic formulae for the shift in the scattering resonances that is caused by a small particle of arbitrary shape. Our formula shows that the perturbation of the scattering resonances can be expressed in terms of the polarization tensor of the small particle. The scattering resonances can be degenerate or even exceptional and the small particle can be plasmonic. Our method is based on pole-pencil decompositions of the volume integral operator associated with the radiating dielectric cavity problem. The new techniques introduced in this chapter can not be easily extended to the transverse magnetic case considered in Chapter 6, mainly due to the hyper-singular character of the associated volume-integral operator.

The chapter is organized as follows. In Section 7.1, we characterize the scattering resonances of dielectric cavities in terms of the spectrum of a volume integral operator. In Section 7.2, using the method of pole-pencil decompositions (see, for instance, [9, 14]), we derive the leading-order term in the shift of the scattering resonances of an open dielectric cavity due to presence of internal particles. In Section 7.3, using a Lippmann-Schwinger representation formula for the Green's function associated with the open cavity, we generalize the formula obtained in Section 7.2 to the case of external particles. In Section 7.4, we consider the perturbation of an open dielectric cavity by plasmonic nanoparticles. The formula obtained for the perturbation of the frequencies shows a strong enhancement in the frequency shift in the case of plasmonic nanoparticles. In Section 7.5, we examine the case of exceptional points and reformulate the search for scattering resonances as a search for the roots of a polynomial.

7.1 Scattering resonances of a dielectric cavity

Let Ω be a domain in $\mathbb{R}^d$ for $d = 2, 3$, with smooth boundary $\partial\Omega$. Consider the operator $\Delta + \varepsilon\mu_m\omega^2$ where $\omega \in \mathbb{C}$ is the frequency, $\varepsilon \equiv \tau\varepsilon_c + \varepsilon_m$ inside Ω and $\varepsilon \equiv \varepsilon_m$ outside Ω. Here, $\varepsilon_c, \varepsilon_m, \mu_m$ and τ are positive constants.

Let Γ_m be the outgoing (i.e., subject to the Sommerfeld radiation condition (1.5)) fundamental solution of $\Delta + \varepsilon_m\mu_m\omega^2$ in free space, and let G be the outgoing fundamental solution of $\Delta + \varepsilon\mu_m\omega^2$ in free space. Let

$$K_\Omega^\omega : u \in \mathrm{L}^2(\Omega) \mapsto -\int_\Omega u(y)\Gamma_m(\,\cdot\,, y; \omega)dy \in \mathrm{L}^2(\Omega).$$

The operator $K_\Omega^\omega : \mathrm{L}^2(\Omega) \to \mathrm{L}^2(\Omega)$ is of Hilbert-Schmidt type, and thus compact. Therefore, its spectrum is

$$\sigma(K_\Omega^\omega) = \{0, \lambda_1(\omega), \lambda_2(\omega), \dots, \lambda_j(\omega), \dots\},$$

where $|\lambda_j(\omega)| \geq |\lambda_{j+1}(\omega)|$, $\lambda_j(\omega) \to 0$ as $j \to +\infty$ and $\{0\} = \sigma(K_\Omega^\omega) \setminus \sigma_p(K_\Omega^\omega)$ with $\sigma_p(K_\Omega^\omega)$ being the point spectrum. Note that, due to the uniqueness of the exterior Helmholtz problem, the imaginary part $\Im\lambda_j(\omega)$ must be non-zero for all j and $\omega \in \mathbb{R}$. Let H_j be the generalized eigenspace associated with $\lambda_j(\omega)$. Then, from [24, Lemma 3.5], we have that $\mathrm{L}^2(\Omega)$ is the closure of the union of all generalized eigenspaces H_j in L^2-norm.

Let ω_0 and τ be such that there exists a j_0 such that

$$1 - \omega_0^2\tau\varepsilon_c\mu_m\lambda_{j_0}(\omega_0) = 0. \tag{7.1}$$

We call such an $\omega_0 \in \mathbb{C}$ (with $\Im\omega_0 \neq 0$) a scattering resonance of the open dielectric cavity Ω. Moreover, for τ large enough, (7.1) has solutions. Furthermore, assume that for ω in a complex neighborhood of ω_0, the following assumptions hold:

(i) We have

$$1 - \omega^2\tau\varepsilon_c\mu_m\lambda_{j_0}(\omega) = R(\omega)(\omega - \omega_0),$$

where $R(\omega_0) \neq 0$ and $\omega \mapsto R(\omega)$ is analytic;

(ii) The generalized eigenspace $H_{j_0}(\omega)$ is of dimension 1.

If both of these assumptions are satisfied, then we say that the scattering resonance ω_0 is non-exceptional.

Assume that ω_0 is a non-exceptional scattering resonance. As a consequence of classic expansion theorems for fundamental solutions (see [37, *expansion theorems*]) we have that there exists a complex neighborhood $V(\omega_0)$ of ω_0 such that for ω in $V(\omega_0) \setminus \{\omega_0\}$,

$$\begin{aligned} G(x, y; \omega) \quad &= \quad \Gamma_m(x, y; \omega) + c_{j_0}(\omega) \frac{e_{j_0}(x; \omega) e_{j_0}(y; \omega)}{\omega - \omega_0} \\ &\qquad + \text{some function that is smooth in } x, y \text{ and analytic in } \omega, \end{aligned} \tag{7.2}$$

where e_{j_0} spans H_{j_0}, $\|e_{j_0}\|_{\mathrm{L}^2(\Omega)} = 1$, and $\omega \mapsto e_{j_0}(\,\cdot, \omega)$ and $\omega \mapsto c_{j_0}(\omega)$ are analytic in $V(\omega_0)$. Note that $e_{j_0}(y; \omega_0)$ is the restriction to Ω of the eigenmode associated with the scattering resonance ω_0.

7.2 Shift of resonances by internal particles

Let D be a domain compactly contained in Ω, such that $D = z + \delta B$, where δ is the characteristic size of D, z is its location, and B is a smooth bounded domain containing the origin. We suppose that D has a different magnetic permeability from μ_m, and consider the operator

$$\nabla \cdot \frac{1}{\mu} \nabla + \varepsilon \omega^2,$$

where $\mu = \mu_c$ in D and $\mu = \mu_m$ outside D.

As $\delta \to 0$, we seek an ω_δ in a neighborhood of ω_0 such that there exists a non-trivial solution to

$$\Big(\nabla \cdot \frac{1}{\mu} \nabla + \varepsilon \omega_\delta^2\Big) u = 0,$$

subject to the Sommerfeld radiation condition. Integrating by parts and using the radiation condition, it is easy to show that the solution to the above problem admits the following Lippmann-Schwinger representation formula:

$$u(x) = \gamma \int_D \nabla u(y) \cdot \nabla G(x, y; \omega_\delta)\, dy \quad \text{for all } x \in \mathbb{R}^d,$$

where $\gamma = (1/\mu_c) - (1/\mu_m)$. Consider the volume integral operator

$$T_D^\omega : v \mapsto \nabla_x \int_D v(y) \cdot \nabla G(x, y; \omega)\, dy,$$

where the integral on the right hand side is intended in the principal value sense. Then the operator $T_D^\omega : \mathrm{L}^2(D)^d \to \mathrm{L}^2(D)^d$ is well-defined (see, for instance, [17, Appendix B] and references therein).

We seek ω_δ such that there is a non-trivial $v \in \mathrm{L}^2(D)^d$ satisfying

$$\left(I - \gamma T_D^{\omega_\delta}\right)[v] = 0, \tag{7.3}$$

where I denotes the identity operator. Hence, as the characteristic size δ of D goes to zero, we seek ω_δ in a neighborhood of ω_0 such that $1/\gamma$ is an eigenvalue of $T_D^{\omega_\delta}$.

From the pole-pencil decomposition (7.2) of G, we have

$$\nabla \int_D v \cdot \nabla G = \nabla \int_D v \cdot \nabla \Gamma_m + \frac{c_{j_0}(\omega)}{\omega - \omega_0}\Big(\int_D v \cdot \nabla e_{j_0}\, dy\Big)\nabla e_{j_0}(x;\omega) + R[v],$$

where $R : \mathrm{L}^2(D)^d \to \mathrm{L}^2(D)^d$ is an operator with smooth kernel that is analytic in $\omega \in V(\omega_0)$. Let

$$N_D^\omega : v \mapsto \nabla_x \int_D v(y) \cdot \nabla \Gamma_m(x, y; \omega) dy.$$

Then, it follows that

$$(I/\gamma - T_D^\omega)[v] = (I/\gamma - N_D^\omega)[v] - \frac{c_{j_0}(\omega)}{\omega - \omega_0}(v, \nabla e_{j_0})\nabla e_{j_0} + R[v],$$

where $(\,\cdot\,,\,\cdot\,)$ denotes the L^2 real scalar product on D and I is the identity operator.

From [36, 46], it is known that $N_D^\omega|_W : W \longrightarrow W$ is a compact operator, where W is the space of gradients of harmonic functions in D. Moreover, the spectrum of $N_D^\omega|_W$ is discrete and the associated eigenfunctions form a basis of W.

Let $L = I/\gamma - N_D^{\omega=0}$. Then, (7.3) can be rewritten as

$$L[v] - \frac{c_{j_0}(\omega)}{\omega - \omega_0}(v, \nabla e_{j_0})\nabla e_{j_0} + \widetilde{R}[v] = 0,$$

where $\widetilde{R} : \mathrm{L}^2(D)^d \to \mathrm{L}^2(D)^d$ is an operator with smooth kernel that is analytic in $\omega \in V(\omega_0)$. Therefore, since for μ_c large enough L is invertible,

$$v - \frac{c_{j_0}(\omega)}{\omega - \omega_0}(v, \nabla e_{j_0})L^{-1}[\nabla e_{j_0}] + L^{-1}\widetilde{R}[v] = 0.$$

So, since

$$||L^{-1}\widetilde{R}||_{\mathcal{L}(\mathrm{L}^2(D)^d, \mathrm{L}^2(D)^d)} = o(1) \quad \text{as } \delta \to 0,$$

(see [17, Lemma 4.2] and [14]), the term $L^{-1}\widetilde{R}[v]$ can be neglected, and we have the leading-order asymptotic approximation

$$\omega_\delta - \omega_0 \sim c_{j_0}(\omega_0)(L^{-1}[\nabla e_{j_0}], \nabla e_{j_0}).$$

Moreover, from [17, Proposition 3.1], it follows that

$$(L^{-1}[\nabla e_{j_0}], \nabla e_{j_0}) \sim \delta^d M(\mu_m/\mu_c, B)\nabla e_{j_0}(z;\omega_0)\cdot\nabla e_{j_0}(z;\omega_0),$$

where M is the polarization tensor given by (1.11).

In conclusion, the following proposition holds.

Proposition 7.1. *As $\delta \to 0$, we have*

$$\omega_\delta - \omega_0 \sim \delta^d c_{j_0}(\omega_0) M(\mu_m/\mu_c, B)\nabla e_{j_0}(z;\omega_0)\cdot\nabla e_{j_0}(z;\omega_0). \tag{7.4}$$

7.3 Shift of resonances by external particles

Now consider the case where the particle is outside Ω. Again by integration by parts and the radiation conditions, we obtain the following Lippmann-Schwinger representation formula for G:

$$G(x,z;\omega) = \Gamma_m(x,z;\omega) - \omega^2\tau\varepsilon_c\mu_m\int_\Omega G(z,z';\omega)\Gamma_m(z',x;\omega)\,dz', \tag{7.5}$$

for $x, z\in\mathbb{R}^d, x\neq z$. On the other hand, for x outside Ω and z inside Ω, using (7.2) we obtain,

$$\begin{aligned} G(x,z;\omega) = \Gamma_m(x,z;\omega) - \frac{\omega^2\tau\varepsilon_c\mu_m c_{j_0}(\omega)}{\omega-\omega_0} e_{j_0}(z;\omega)\left(\int_\Omega e_{j_0}(z';\omega)\Gamma_m(z',x;\omega)\,dz'\right) \\ + \text{ a function that is smooth in } x, z, \text{ and analytic in } \omega. \end{aligned} \tag{7.6}$$

For x, z both outside Ω, $x\neq z$, plugging (7.6) back into (7.5), we arrive at

$$\begin{aligned} G(x,z;\omega) = \Gamma_m(x,z;\omega) + \frac{c_{j_0}(\omega)}{\omega-\omega_0} g_{j_0}(z;\omega) g_{j_0}(x;\omega) \\ + \text{ a function that is smooth in } x, z, \text{ and analytic in } \omega, \end{aligned}$$

where we defined

$$g_{j_0}(\,\cdot\,;\omega) = \omega^2\tau\varepsilon_c\mu_m\int_\Omega e_{j_0}(z';\omega)\Gamma_m(z',\,\cdot\,;\omega)\,dz'.$$

Note that g_{j_0}, defined by the above formula for all $x\in\mathbb{R}^d$, is the eigenmode associated with the scattering resonance ω_0, and it coincides with $e_{j_0}(x;\omega_0)$ on Ω.

Analogously to the calculations in the previous section, we have

$$v - \frac{c_{j_0}(\omega)}{\omega-\omega_0}(v, \nabla g_{j_0}) L^{-1}[\nabla g_{j_0}] + L^{-1}R[v] = 0,$$

for some operator R with smooth kernel that is analytic in ω in $V(\omega_0)$. Therefore, analogously to (7.4), the following asymptotic expansion holds.

Proposition 7.2. *As $\delta \to 0$, we have*

$$\omega_\delta - \omega_0 \sim \delta^d c_{j_0}(\omega_0) M(\mu_m/\mu_c, B) \nabla g_{j_0}(z;\omega_0) \cdot \nabla g_{j_0}(z;\omega_0). \tag{7.7}$$

7.4 Shift of resonances by plasmonic particles

Suppose now that D is a plasmonic particle, i.e., μ_c depends on ω and for a discrete set of frequencies ω, called plasmonic resonances, the polarization tensor is singular, see [8, 18, 21]. In this case, the scattering resonance problem consists in finding ω such that there is a non-trivial solution v to

$$L(\omega)[v] - \frac{c_{j_0}(\omega)}{\omega - \omega_0}(v, \nabla e_{j_0}) \nabla e_{j_0} + R[v] = 0,$$

where $L(\omega) = I/\gamma(\omega) - N_D^{\omega=0}$. The operator L is not invertible at plasmonic resonances. Using the Drude model for the permeability, we have $\mu_c(\omega) = \mu_m(1 - \omega_p^2/\omega^2)$, where ω_p is the volume plasma frequency. Let (λ_j, φ_j) be an eigenvalue-eigenfunction pair of L. Then

$$v - \frac{c_{j_0}(\omega)}{\omega - \omega_0} \frac{(v, \nabla e_{j_0})(\nabla e_{j_0}, \varphi_j)\varphi_j}{\lambda(\omega) - \lambda_j} = 0,$$

and thus,

$$1 - \frac{c_{j_0}(\omega_0)}{\omega - \omega_0} \frac{(\nabla e_{j_0}, \varphi_j)^2}{\lambda(\omega) - \lambda_j} = 0.$$

So, we arrive at the following proposition.

Proposition 7.3. *As $\delta \to 0$, we have*

$$(\omega_\delta - \omega_0)(\lambda(\omega_\delta) - \lambda_j) \sim c_{j_0}(\omega_0)(\nabla e_{j_0}, \varphi_j)^2.$$

Note that if $\lambda(\omega) - \lambda_j = O(\omega - \omega_0)$ for ω close to ω_0, then we obtain

$$(\omega_\delta - \omega_0)^2 \sim c_{j_0}(\omega_0)(\nabla e_{j_0}(\cdot;\omega_0), \varphi_j)^2,$$

Hence, we have a significant shift in the scattering resonances if the particle D is plasmonic and resonant near or at the frequency ω_0. This anomalous effect has been observed in [92].

7.5 Asymptotic analysis near exceptional points

In this section, we examine the asymptotic behavior of an exceptional scattering resonance for a particular form of the Green function. These exceptional resonances are due to the non-Hermitian character of the operator T_D^ω, see [24, 88]. For simplicity and in view of the Jordan-type decomposition of the operator T_D^ω established in [24], we assume that, for ω near ω_0, $G(x,y;\omega)$ behaves like

$$G(x,y;\omega)=\Gamma_m(x,y;\omega)+c_1(\omega)\frac{h^{(1)}(x;\omega)h^{(1)}(y;\omega)}{\omega-\omega_0}+c_2(\omega)\frac{h^{(2)}(x;\omega)h^{(2)}(y;\omega)}{(\omega-\omega_0)^2}+R(\omega), \tag{7.8}$$

for two functions $h^{(1)}$ and $h^{(2)}$ in $\mathrm{L}^2(D)$. In this simple case, we characterize the shift of the scattering resonance ω_0 due to the small particle D, which is assumed for simplicity to be non-plasmonic.

Following the same arguments as those in the previous sections, we seek a non-trivial v such that

$$L[v]-c_1(\omega)\frac{(v,\nabla h^{(1)})}{\omega-\omega_0}\nabla h^{(1)}-c_2(\omega)\frac{(v,\nabla h^{(2)})}{(\omega-\omega_0)^2}\nabla h^{(2)}=0,$$

or equivalently,

$$v-c_1(\omega)\frac{(v,\nabla h^{(1)})}{\omega-\omega_0}L^{-1}[\nabla h^{(1)}]-c_2(\omega)\frac{(v,\nabla h^{(2)})}{(\omega-\omega_0)^2}L^{-1}[\nabla h^{(2)}]=0.$$

By multiplying the above equation by $\nabla h^{(1)}$ and $\nabla h^{(2)}$, respectively, and integrating by parts over D, we obtain the following system of equations:

$$\begin{cases} (v,\nabla h^{(1)})\left(1-c_1(\omega)\dfrac{(L^{-1}[\nabla h^{(1)}],\nabla h^{(1)})}{\omega-\omega_0}\right)=c_2(\omega)(v,\nabla h^{(2)})\dfrac{(L^{-1}[\nabla h^{(2)}],\nabla h^{(1)})}{(\omega-\omega_0)^2}, \\ (v,\nabla h^{(2)})\left(1-c_2(\omega)\dfrac{(L^{-1}[\nabla h^{(2)}],\nabla h^{(2)})}{(\omega-\omega_0)^2}\right)=c_1(\omega)(v,\nabla h^{(1)})\dfrac{(L^{-1}[\nabla h^{(1)}],\nabla h^{(2)})}{\omega-\omega_0}. \end{cases}$$

Therefore, the following result holds.

Proposition 7.4. *Assume that the decomposition (7.8) holds for ω near ω_0. Then the perturbed scattering resonance problem (due to the particle D) can be reformulated as a search for ω near ω_0 such that the matrix*

$$\begin{pmatrix} 1-c_1(\omega)\dfrac{(L^{-1}[\nabla h^{(1)}],\nabla h^{(1)})}{\omega-\omega_0} & -c_2(\omega)\dfrac{(L^{-1}[\nabla h^{(2)}],\nabla h^{(1)})}{(\omega-\omega_0)^2} \\ c_1(\omega)\dfrac{(L^{-1}[\nabla h^{(1)}],\nabla h^{(2)})}{\omega-\omega_0} & 1-c_2(\omega)\dfrac{(L^{-1}[\nabla h^{(2)}],\nabla h^{(2)})}{(\omega-\omega_0)^2} \end{pmatrix}$$

is singular.

In conclusion, in this chapter we derived the leading-order term in the shift of scattering resonances of a radiating dielectric cavity due to the presence of small particles. We were able also to give a characterization of the shift due to small particles near an exceptional scattering resonance in a specific case. However, developing a general theory near exceptional frequencies remains a challenging open problem.

Chapter 8

Scattering of highly refractive particles

Nanoscale optics is usually associated with plasmonic resonant structures made of metals such as gold or silver. Plasmonic resonances of nanoparticles can be treated as an eigenvalue problem for the Neumann-Poincaré operator, see [8, 17, 18, 21]. However, plasmonic structures suffer from the high losses inherent in metals and dissipation due to heating. Recent developments in nanoscale optical physics have led to a new branch of nanophotonics focused on the manipulation of optically induced subwavelength resonances in dielectric nanoparticles with high refractive indices [67, 102, 103]. Resonant high-index dielectric nano-structures form new building blocks which can be used to realize unique functionalities and novel photonic devices [67]. Their study has been established as a new research direction in nanophotonics. Nevertheless, despite strong experimental efforts, mathematical modeling of resonant high-index nanoparticles remains limited.

In this chapter, we consider a dielectric high-index nanoparticle of arbitrary shape and characterize its subwavelength resonances in terms of the eigenvalues of the Newtonian potential associated with its shape. Our formula is closely related to the one established in [78]. Then, we provide an asymptotic formula for the field scattered by a dielectric nanoparticle and estimate the scattering enhancement near its resonant frequencies. We also consider the hybridization phenomenon of a dimer consisting of high refractive index dielectric nanoparticles.

Our results in this chapter provide a new mathematical framework for the analysis of resonant dielectric nanoparticles. They allow quick computations of estimates of resonant frequencies and the design of dielectric nanoparticles that resonate at specified frequencies. They can also be applied in the design of dielectric metamaterials [61, 102, 103].

8.1 Derivation of asymptotic estimates

Let D be a domain contained in $\mathbb{R}^d$, for $d = 2$ or 3, such that $D = z + \delta B$, where δ is its characteristic size, z its location, and B is a smooth bounded domain containing the origin. Let ω denote the frequency, let $\varepsilon \equiv \tau\varepsilon_c + \varepsilon_m$ inside D and $\varepsilon \equiv \varepsilon_m$ outside D. Here, $\varepsilon_c, \varepsilon_m$, and τ are positive constants. Let E^{in} be an incident plane wave with frequency ω.

Consider the Helmholtz equation

$$\begin{cases} (\Delta + \omega^2\varepsilon)E = 0 \quad \text{in } \mathbb{R}^d, \\ E - E^{\text{in}} \text{ satisfies the Sommerfeld radiation condition.} \end{cases}$$

From

$$(\Delta + \omega^2\varepsilon_m)(E - E^{\text{in}}) = -\omega^2\tau\varepsilon_c E\chi_D \quad \text{in } \mathbb{R}^d,$$

where χ_D is the characteristic function of D, it follows that the following Lippman-Schwinger representation formula holds:

$$(E - E^{\text{in}})(x) = -\omega^2\tau\varepsilon_c \int_D E(y)\Gamma_m(x, y; \omega)dy \quad \text{for } x \in \mathbb{R}^d, \tag{8.1}$$

where Γ_m is the outgoing (i.e., subject to the Sommerfeld radiation condition) fundamental solution of $\Delta + \varepsilon_m\omega^2$ in free space.

Let the volume integral operator K_D^ω be defined by

$$K_D^\omega : E \in \mathrm{L}^2(D) \mapsto -\int_D E(y)\Gamma_m(x, y; \omega)dy \in \mathrm{L}^2(D).$$

It is well known that, due to the weak singularity of the fundamental solution, K_D^ω is compact. When $|\tau\omega^2\varepsilon_c K_D^\omega| < 1$, then $I - \tau\omega^2\varepsilon_c K_D^\omega$ is invertible, so (8.1) can be rewritten as

$$E(x) = (I - \tau\omega^2\varepsilon_c K_D^\omega)^{-1}[E^{\text{in}}](x) \quad \text{for all } x \in D, \tag{8.2}$$

where I denotes the identity operator.

Assume that the characteristic size δ of the particle D is much smaller than the wavelength $2\pi/(\omega\sqrt{\varepsilon_m})$, and let $\omega \to 0$. The subwavelength resonance problem is then to find an $\omega \in \mathbb{C}$ close to 0 such that $(I - \tau\omega^2\varepsilon_c K_D^\omega)^{-1}$ is singular, see [24]. Such an ω would be a subwalength resonance for the high refractive index dielectric particle D.

By expanding in Taylor series the fundamental solution we obtain the following result.

Lemma 8.1. *Let $d = 3$. Let $K_D^{(0)}$ be the Newtonian potential on D, i.e., the operator defined by*

$$K_D^{(0)}[E](x) = -\int_D E(y)\Gamma_0(|x-y|)\,dy \quad \textit{for } x \in D.$$

The operator K_D^ω can be rewritten as

$$K_D^\omega = \sum_{i=0}^{\infty} \omega^i K_D^{(i)}, \tag{8.3}$$

where the series converges in operator norm if ω is small enough.

Let $A_i = \tau\omega^2\varepsilon_c K_D^{(i)}$. By expanding in Neumann series, we have

$$\begin{aligned}
\Big(I - A_0 - \sum_{i=1}^{\infty}\omega^i A_i\Big)^{-1} &= \Big(I - (I-A_0)^{-1}\sum_{i=1}^{\infty}\omega^i A_i\Big)^{-1}(I-A_0)^{-1} \\
&= \sum_{k=0}^{\infty}\Big((I-A_0)^{-1}\sum_{i=1}^{\infty}\omega^i A_i\Big)^k (I-A_0)^{-1} \\
&= (I-A_0)^{-1} + (I-A_0)^{-1}\omega A_1 (I-A_0)^{-1} + O(\omega^3). \quad (8.4)
\end{aligned}$$

Recall that $K_D^{(0)} : \mathrm{L}^2(D) \to \mathrm{L}^2(D)$ is a compact, self-adjoint operator. Let λ_0 be an eigenvalue of $K_D^{(0)}$ associated with the eigenfunction ϕ_0. We remark that the eigenvalues of $K_D^{(0)}$ are positive. For the analysis of the spectrum of the Newtonian potential, we refer the reader, for instance, to [62].

Let ω_0 be a frequency at which $I - A_0$ becomes singular. In particular, let

$$\omega_0 = 1/\sqrt{\tau\varepsilon_c\lambda_0}. \tag{8.5}$$

Note that ω_0 is small only for τ large enough. This shows that subwavelength resonances occur only for particles with high refractive indices.

For ω near ω_0, we have, by a pole-pencil operator decomposition, that

$$(I-A_0)^{-1}[\psi] = \frac{(\psi,\phi_0)\phi_0}{1-\tau\omega^2\varepsilon_c\lambda_0}.$$

Therefore considering only the first two terms in the expansion (8.4), we obtain from (8.2) that an approximation of the resonance must satisfy

$$\frac{(E^{\mathrm{in}},\phi_0)\phi_0}{1-\tau\omega^2\varepsilon_c\lambda_0} + \tau\omega^3\varepsilon_c\frac{(K_D^{(1)}[\phi_0],\phi_0)}{(1-\tau\omega^2\varepsilon_c\lambda_0)^2}(E^{\mathrm{in}},\phi_0)\phi_0 = 0,$$

where $(\,\cdot,\cdot\,)$ denotes the scalar product on $\mathrm{L}^2(D)$.

Therefore we have the following approximation for the subwavelength resonance.

Proposition 8.2. *Let $d=3$. Then, the $O(\omega^4)$-approximation of the subwavelength resonant frequency ω_{res} of the dielectric particle D satisfies*

$$1-\tau\omega_{\mathrm{res}}^2\varepsilon_c\lambda_0 = -\tau\omega_{\mathrm{res}}^3\varepsilon_c(K_D^{(1)}[\phi_0],\phi_0).$$

Note that, in three dimensions,

$$K_D^{(1)}[\phi] = -\mathrm{i}\frac{\sqrt{\varepsilon_m}}{4\pi}\int_D \phi\, dy \quad \text{for all } \phi\in \mathrm{L}^2(D).$$

Therefore, ω_{res} satisfies

$$1-\tau\omega_{\mathrm{res}}^2\varepsilon_c\lambda_0 = \frac{\mathrm{i}\tau}{4\pi}\omega_{\mathrm{res}}^3\sqrt{\varepsilon_m}\varepsilon_c\Big(\int_D \phi_0\, dy\Big)^2.$$

Since ω_{res} is close to ω_0, by approximating $\omega_{\mathrm{res}}^3\simeq\omega_0^3$, and since by definition $\tau\varepsilon_c\lambda_0 = 1/\omega_0^2$, we obtain

$$1-\frac{\omega_{\mathrm{res}}^2}{\omega_0^2} = \frac{\mathrm{i}\tau}{4\pi}\omega_0^3\sqrt{\varepsilon_m}\varepsilon_c\Big(\int_D \phi_0\, dy\Big)^2.$$

Proposition 8.3. *Let $d=3$. Let ω_0 be defined by (8.5), where λ_0 is an eigenvalue of the Newtonian potential $K_D^{(0)}$. Assume that $\omega_0\ll 1$. Then, an approximation of the subwavelength resonant frequency of the dielectric particle D can be computed as*

$$\omega_{\mathrm{res}} = \omega_0 - \frac{\mathrm{i}}{8\pi}\frac{\omega_0^2}{\lambda_0}\sqrt{\varepsilon_m}\Big(\int_D \phi_0\, dy\Big)^2.$$

By using the Lippman-Schwinger representation formula (8.1), we can also rewrite

$$\begin{aligned}E(x)-E^{\mathrm{in}}(x) \simeq\ & -\omega^2\tau\varepsilon_c\Gamma_m(x-z;\omega)\frac{(E^{\mathrm{in}},\phi_0)(\int_D\phi_0)}{1-\tau\omega^2\varepsilon_c\lambda_0}\\ & +\tau\omega^3\varepsilon_c\frac{(K_D^{(1)}[\phi_0],\phi_0)(E^{\mathrm{in}},\phi_0)(\int_D\phi_0)}{(1-\tau\omega^2\varepsilon_c\lambda_0)^2}.\end{aligned}$$

By plugging the expression for ω_{res} from Proposition 8.2 we obtain the following approximation.

Proposition 8.4. *For ω near the resonant frequency ω_{res}, the following monopole approximation of the dielectric nanoparticle D holds:*

$$E(x)-E^{\mathrm{in}}(x) \simeq -\frac{\lambda_0\Big(\frac{\omega_{\mathrm{res}}^2}{\omega^2}-1\Big)-\mathrm{i}\frac{\sqrt{\varepsilon_m}}{4\pi}(\int_D\phi_0)^2\Big(\omega-\frac{\omega_{\mathrm{res}}^3}{\omega^2}\Big)}{\Big(\lambda_0\Big(\frac{\omega_{\mathrm{res}}^2}{\omega^2}-1\Big)-\mathrm{i}\frac{\sqrt{\varepsilon_m}}{4\pi}(\int_D\phi_0)^2\frac{\omega_{\mathrm{res}}^3}{\omega^2}\Big)^2}(E^{\mathrm{in}},\phi_0)_{\mathrm{L}^2(D)}\Gamma_m(x-z;\omega), \tag{8.6}$$

for $|x-z|\gg 2\pi/(\omega\sqrt{\varepsilon_m})$.

Now, we consider the two-dimensional case. From the asymptotic expansion of the Hankel function $H_0^{(1)}$ of the first kind of order zero:

$$H_0^{(1)}(s) = \frac{2i}{\pi}\sum_{m=0}^{\infty}(-1)^m \frac{s^{2m}}{2^{2m}(m!)^2}\Big(\log(\gamma s) - \sum_{j=1}^{m}\frac{1}{j}\Big),$$

where $2\gamma = \exp(\widetilde{\gamma} - \mathrm{i}\pi/2)$ with $\widetilde{\gamma}$ being the Euler-Mascheroni constant (see, for instance, [20]), it follows that

$$K_D^{\omega}[E] = -\frac{1}{2\pi}(\log(\omega\gamma))\int_D E(y)\,dy + K_D^{(0)} + O(\omega^2\log\omega) \quad \text{as } \omega \to 0, \tag{8.7}$$

where $K_D^{(0)}$ is the Newtonian potential in dimension two, that is, the operator defined on $\mathrm{L}^2(D)$ by

$$K_D^{(0)}[E](x) = \int_D E(y)\Gamma(x-y)\,dy \quad \text{for } x \in D,$$

with Γ being the fundamental solution of the Laplacian in $\mathbb{R}^2$.

Expanding K_D^{ω} as in (8.4) and following the same calculations, we obtain the following characterization of subwavelength resonant frequencies in the two-dimensional case.

Proposition 8.5. *Let $d = 2$. Then, the $o(\omega^4)$-approximation of the subwavelength resonant frequencies ω_{res} of the dielectric particle D satisfies*

$$1 - \tau\omega_{\mathrm{res}}^2\varepsilon_c\lambda_0 - \frac{\tau\varepsilon_c}{2\pi}\omega_{\mathrm{res}}^2\log(\gamma\omega_{\mathrm{res}})\Big(\int_D \phi_0\,dy\Big)^2 = O(\omega^4\log\omega).$$

8.2 Hybridization of subwavelength resonances for a dimer of dielectric nanoparticles

Consider a dimer of two identical particles D_1 and D_2 with the same dielectric parameter as in the above section. Then the field $E - E^{\mathrm{in}}$ scattered by the two particles has the following representation formula:

$$(E - E^{\mathrm{in}})(x) = -\omega^2\tau\varepsilon_c\Big(\int_{D_1} E(y)\Gamma_m(x-y;\omega)dy + \int_{D_2} E(y)\Gamma_m(x-y;\omega)dy\Big). \tag{8.8}$$

Define the operators $K_{D_i}^{\omega}$ and R_{D_i,D_j}^{ω} for $i,j = 1,2$, by

$$K_{D_i}^{\omega} : E|_{D_i} \in \mathrm{L}^2(D_i) \mapsto -\int_{D_i} E(y)\Gamma_m(x-y;\omega)dy\big|_{D_i} \in \mathrm{L}^2(D_i),$$

and

$$R_{D_i,D_j}^{\omega} : E|_{D_i} \in \mathrm{L}^2(D_i) \mapsto -\int_{D_i} E(y)\Gamma_m(x-y;\omega)dy\big|_{D_j} \in \mathrm{L}^2(D_j).$$

Then, from (8.8) we obtain the following system of operator equations:

$$\begin{pmatrix} 1-\tau\omega^2\varepsilon_c K^{\omega}_{D_1} & -\tau\omega^2\varepsilon_c R^{\omega}_{D_2,D_1} \\ -\tau\omega^2\varepsilon_c R^{\omega}_{D_1,D_2} & 1-\tau\omega^2\varepsilon_c K^{\omega}_{D_2} \end{pmatrix} \begin{pmatrix} E|_{D_1} \\ E|_{D_2} \end{pmatrix} = \begin{pmatrix} E^{\text{in}}|_{D_1} \\ E^{\text{in}}|_{D_2}. \end{pmatrix} \tag{8.9}$$

The scattering resonance problem is to find ω such that the operator in (8.9) is singular. Note that here we have a coupled system of subwavelength resonators. As in [9, 10], the subwavelength resonant frequency ω_{res} is hybridized into two subwavelength resonant frequencies $\omega_{\text{res}}^{\pm}$ approximately given by

$$\omega_{\text{res}}^{\pm} = \omega_0 \pm \frac{1}{2}\tau\omega_0^3\varepsilon_c\sqrt{(R^{\omega_{\text{res}}}_{D_1,D_2}[\phi_0^{(1)}],\phi_0^{(2)})(R^{\omega_{\text{res}}}_{D_2,D_1}[\phi_0^{(2)}],\phi_0^{(1)})}, \tag{8.10}$$

where $\phi_0^{(i)}$, for $i=1,2$, is the eigenfunction associated to the eigenvalue λ_0 of the Newtonian potential of D_i. Moreover, in the far-field, the dimer of dielectric particles behaves as the sum of a monopole and a dipole.

In conclusion, in this chapter we provided a mathematical model of resonant high-index nanoparticles. Our results can be used for the analysis, design, and manipulation of resonant dielectric nano-structures and their use as metamaterials. Following [11], we believe that formula (8.6) can be generalized to the time-domain, in order to characterize the temporal response of resonant dielectric nanoparticles and accelerate the computations of the responses of subwavelength dielectric resonators [42, 101].

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