



Perturbations of the scattering resonances of an open cavity by small particles. Part II: The transverse electric polarization case

H. Ammari and A. Dabrowski and B. Fitzpatrick and P. Millien

Research Report No. 2018-39

October 2018 Latest revision: January 2019

Seminar für Angewandte Mathematik Eidgenössische Technische Hochschule CH-8092 Zürich Switzerland

Perturbations of the scattering resonances of an open cavity by small particles. Part II: The transverse electric polarization case

Habib Ammari* Alexander Dabrowski* Brian Fitzpatrick[†]
Pierre Millien[‡]

Abstract

This paper is concerned with the scattering resonances of open cavities. It is a follow-up of [1], where the transverse magnetic polarization was assumed. In that case, using the method of matched asymptotic expansions, the leading-order term in the shifts of scattering resonances due to the presence of small particles of arbitrary shapes was derived and the effect of radiation on the perturbations of open cavity modes was characterized. The derivations were formal. In this paper, we consider the transverse electric polarization and prove a small-volume formula for the shifts in the scattering resonances of a radiating dielectric cavity perturbed by small particles. We show a strong enhancement in the frequency shift in the case of subwavelength particles with dipole resonances. We also consider exceptional scattering resonances and perform small-volume asymptotic analysis near them. A significant observation is the large-amplitude splitting of exceptional scattering resonances induced by small particles. Our method in this paper relies on pole-pencil decompositions of volume integral operators.

Mathematics Subject Classification (MSC2000). 35R30, 35C20.

Keywords. Open dielectric resonator, shift of scattering resonances, exceptional scattering resonances, splitting of scattering resonances, subwavelength resonant nanoparticles, pole-pencil decomposition.

1 Introduction

In this paper, which is a follow-up of [1], we consider dielectric radiating cavities [10,12,20] and rigorously obtain asymptotic formulas for the shifts in the scattering resonances that are due to a small particle of arbitrary shape. Our formula shows that the perturbations of the scattering resonances are proportional to the polarization tensor of the small particle. Therefore, the shift of the scattering frequencies induced by the small particle is of the order of the particle's volume. When the particle is excited near its resonant frequencies, its polarization tensor blows up and consequently, as shown in this paper, an anomalous shift of the scattering resonances can be observed when the resonant particle is coupled to the cavity modes. We also consider

^{*}Department of Mathematics, ETH Zürich, Rämistrasse 101, CH-8092 Zürich, Switzerland (habib.ammari@math.ethz.ch, alexander.dabrowski@sam.math.ethz.ch).

[†]ESAT - STADIUS, Stadius Centre for Dynamical Systems, Signal Processing and Data Analytics, Kasteelpark Arenberg 10 - box 2446, 3001 Leuven, Belgium (bfitzpat@esat.kuleuven.be).

[‡]Institut Langevin, 1 Rue Jussieu, 75005 Paris, France (pierre.millien@espci.fr).

the case where the scattering resonances are exceptional. Exceptional scattering resonances can be defined as the poles of the Green's function associated with the radiating cavity which are not simple [9,16]. They owe their existence to the non-hermitian character of the scattering resonance problem [9,16]. Optical cavities that operate at exceptional scattering frequencies can be exploited for enhanced nanoparticle sensing [13,17]. In this paper, we prove that a small particle inside a cavity perturbs the system from its exceptional points, leading to frequency splitting. Moreover, the splitting induced by the particle is of a much larger amplitude than suggested by the particle's volume. In fact, we consider exceptional points of order two and derive a formula for the splitting of such resonances induced by a small particle. We prove that the strength of the splitting of the exceptional scattering frequencies is proportional to the square root of the volume of the particle.

Our method for proving various formulas that describe the shifts in the scattering resonances due to small particles is based on pole-pencil decompositions (see, for instance, [3,5]) of the volume integral operator associated with the radiating dielectric cavity problem.

The new technique introduced in this paper can not be easily extended to the transverse magnetic case considered in [1] due to the hyper-singular character of the associated volume-integral operator.

The paper is organized as follows. In Section 2, we characterize the scattering resonances of dielectric cavities in terms of the spectrum of a volume integral operator. In Section 3, using the method of pole-pencil decompositions, we derive the leading-order term in the shifts of scattering resonances of an open dielectric cavity due to the presence of internal particles. In Section 4, using a Lippmann-Schwinger representation formula for the Green's function associated with the open cavity, we generalize the formula obtained in Section 3 to the case of external particles. In Section 5, we consider the perturbation of an open dielectric cavity by subwavelength resonant particles. The formula obtained for the shifting of the frequencies shows a strong enhancement in the frequency shift in the case of subwavelength resonant particles. In Section 6, we perform an asymptotic analysis for the shift of exceptional scattering resonances. The paper ends with some concluding remarks.

2 Scattering resonances of a dielectric cavity

2.1 Model

We consider the scattering of linearly polarized light by a dielectric cavity in a time-harmonic regime. Let Ω be a bounded domain in \mathbb{R}^d for d=2,3, with smooth boundary $\partial\Omega$. Assume $\varepsilon \equiv \tau \varepsilon_c + \varepsilon_m$ inside Ω and $\varepsilon = \varepsilon_m$ outside Ω , and $\mu = \mu_m$ everywhere. Here, $\varepsilon_c, \varepsilon_m$, and τ are positive constants. Since we are interested in scattering resonances, we look for solutions u of the homogeneous Helmholtz equation at frequency ω :

$$\begin{cases} \Delta u + \omega^2 \varepsilon(x) \mu_m u = 0 & \text{in } \mathbb{R}^d, \\ u \text{ satisfies the outgoing radiation condition.} \end{cases}$$
 (1)

Let Γ_m be the outgoing 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. We define the following integral operator:

Definition 2.1. Let

$$L^{2}(\Omega) \longrightarrow L^{2}(\Omega)$$

$$u \longmapsto K_{\Omega}^{\omega}[u] := -\int_{\Omega} u(y) \Gamma_{m}(\cdot - y; \omega) dy.$$

The following Lippmann-Swchinger representation formula holds:

Proposition 2.2. u is a solution of (1) if and only if u is a solution of

$$(I - \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega}) [u] = 0.$$
 (2)

According to [9], the following spectral decomposition of the operator K_{Ω}^{ω} holds:

Lemma 2.3. The operator K_{Ω}^{ω} is bounded from $L^{2}(\Omega)$ into $H^{2}(\Omega)$. Moreover, it is a Hilbert-Schmidt operator. Therefore, its spectrum is

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

where $|\lambda_j(\omega)| \to 0$ 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.

Remark 2.4. The scattering resonances are precisely the frequencies for which $(\omega^2 \tau \varepsilon_c \mu_m)^{-1}$ belongs to the spectrum of K_{Ω}^{ω} .

Remark 2.5. Note that $\Im \lambda_i(\omega) \neq 0$ for all j and $\omega \in \mathbb{R}$.

Let H_j be the generalized eigenspace associated with $\lambda_j(\omega)$. Then, from [9], it follows that $L^2(\Omega)$ is the closure of $\bigcup_j H_j$.

Lemma 2.6. We have

$$L^2(\Omega) = \overline{\bigcup_j H_j}.$$

Lemma 2.7. Assume that for any j, dim $H_j = 1$, and denote by e_j a unitary basis vector for H_j . Then the functions

$$f_{j,k}(x,y) = e_j(x)e_k(y),$$

form a normal basis for $L^2(\Omega \times \Omega)$. Moreover,

$$\delta(x - y) = \sum_{j} e_j(x)e_j(y).$$

2.2 Pole pencil decomposition of the Green's function

We denote by $G(x, y; \omega)$ the Green's function associated with problem (1), that is, the solution in the sense of distributions of

$$\left(\Delta_x + \omega^2 \varepsilon(x) \mu_m\right) G(x, y, \omega) = \delta_y,$$

satisfying the outgoing radiation condition.

Definition 2.8. In view of Lemma 2.3 and Remark 2.4, we say that ω_0 is a scattering resonance for the open cavity problem if there exists a j_0 such that

$$1 - \omega_0^2 \tau \varepsilon_c \mu_m \lambda_{j_0}(\omega_0) = 0. \tag{3}$$

We say that the scattering resonance ω_0 is a non-exceptional scattering resonance if the following assumptions hold:

(i) We have

$$1 - \omega^2 \tau \varepsilon_c \mu_m \lambda_{i_0}(\omega) = R(\omega)(\omega - \omega_0),$$

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.

Remark 2.9. It is easy to see that for τ large enough, (3) has solutions.

We can now give the following expansion for G when ω is close to a non exceptional scattering resonance. We refer to Appendix A for its proof.

Proposition 2.10. Assume that ω_0 is a non-exceptional scattering resonance. There exists a complex neighborhood $V(\omega_0)$ of ω_0 such that for ω in $V(\omega_0) \setminus \{\omega_0\}$,

$$G(x,y;\omega) = \Gamma_m(x-y;\omega) + c_{j_0}(\omega_0) \frac{e_{j_0}(x;\omega)e_{j_0}(y;\omega)}{\omega - \omega_0} + \widetilde{R}(x,y;\omega), \tag{4}$$

where $\operatorname{vect}(e_{j_0}) = H_{j_0}$. Moreover, $\omega \mapsto \widetilde{R}(x, y; \omega)$, $\omega \mapsto e_{j_0}(\cdot, \omega)$, and $\omega \mapsto c_{j_0}(\omega)$ are all analytic in $V(\omega_0)$, and $(x, y) \mapsto \widetilde{R}(x, y; \omega)$ is smooth.

3 Shift of the scattering resonances by internal small particles

Now let $D \in \Omega$ be a small particle of the form $D = z + \delta B$, 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 material parameter μ_c that is different 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

$$(\nabla \cdot \frac{1}{\mu} \nabla + \varepsilon \omega_{\delta}^2) u = 0, \tag{5}$$

subject to the outgoing radiation condition.

The following asymptotic expansion of ω_{δ} holds.

Proposition 3.1. As $\delta \to 0$, we have

$$\omega_{\delta} - \omega_0 \simeq \delta^d c_{j_0}(\omega_0) M(\mu_m/\mu_c, B) \nabla e_{j_0}(z; \omega_0) \cdot \nabla e_{j_0}(z; \omega_0). \tag{6}$$

Before proving the above result, we state the following useful lemma. We refer to Appendix B for its proof.

Lemma 3.2. Let

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

Then, T_D is a well defined operator from $L^2(D, \mathbb{R}^d)$ into itself.

Proof. (of Proposition 3.1)

The outgoing solution to problem (5) admits the following Lippmann-Schwinger representation formula:

$$u(x) = (\frac{\mu_m}{\mu_c} - 1) \int_D \nabla u(y) \cdot \nabla G(x, y; \omega_\delta) dy$$
 for all $x \in \mathbb{R}^d$.

Let

$$T_D^{\omega}: v \in L^2(D)^d \mapsto \nabla_x \int_D v(y) \cdot \nabla G(x - y; \omega) dy \in L^2(D)^d.$$

The operator T_D^{ω} is well-defined, see, for instance, [6, Appendix B]. Therefore, we seek ω_{δ} such that there is a non-trivial $v \in L^2(D)^d$ satisfying

$$v(x) - (1/\mu_c - 1/\mu_m) T_D^{\omega_\delta}[v](x) = 0$$
 for all $x \in D$,

or equivalently,

$$\left(I - \left(\frac{\mu_m}{\mu_c} - 1\right)T_D^{\omega_\delta}\right)[v] = 0,$$
(7)

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 $1/((\mu_{m}/\mu_{c})-1)$ is an eigenvalue of $T_{D}^{\omega_{\delta}}$.

From the pole-pencil decomposition (4) of G, we have

$$\nabla \int_{D} v \cdot \nabla G = \nabla \int_{D} v \cdot \nabla \Gamma_{m} + \frac{c_{j_{0}}(\omega)}{\omega - \omega_{0}} \left(\int_{D} v \cdot \nabla e_{j_{0}} \, dy \right) \nabla e_{j_{0}}(x; \omega) + R[v],$$

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

$$N_D^{\omega}: v \in L^2(D)^d \mapsto \nabla_x \int_D v(y) \cdot \nabla \Gamma_m(x-y;\omega) dy \in L^2(D)^d.$$

Then, it follows that

$$\frac{1}{\frac{\mu_{m}}{\mu_{c}} - 1} \left(I - (\frac{\mu_{m}}{\mu_{c}} - 1) T_{D}^{\omega} \right) [v] = \left(\frac{I}{\frac{\mu_{m}}{\mu_{c}} - 1} - N_{D}^{\omega} \right) [v] - \frac{c_{j_{0}}(\omega)}{\omega - \omega_{0}} (v, \nabla e_{j_{0}}) \nabla e_{j_{0}} + R[v],$$

where (\cdot, \cdot) denotes the L^2 real scalar product on D.

Let

$$L = 1/((\mu_m/\mu_c) - 1)I - N_D^0, \tag{8}$$

where $N_D^0 := N_D^{\omega=0}$. Then, (7) 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 $\widetilde{R}: L^2(D)^d \to L^2(D)^d$ is an operator with smooth kernel that is analytic in $\omega \in V(\omega_0)$. Now, we make use of the orthogonal decomposition of $L^2(D, \mathbb{R}^d)$ and the spectral analysis of N_D^0 on $L^2(D, \mathbb{R}^d)$ that can be found in [14,15]. More precisely, recall that

$$L^{2}\left(D,\mathbb{R}^{d}\right) = \nabla H_{0}^{1}(D) \oplus H(\text{div }0,D) \oplus W,$$

where $H_0^1(D)$ is the set of H^1 -functions in D with trace zero on ∂D , H(div 0,D) is the space of divergence free L^2 -vector fields and W is the space of gradients of harmonic H^1 functions. Here, H^1 is the set of function in L^2 having their weak derivatives in L^2 . We will use the following lemma:

Lemma 3.3. The operator N_D^0 is a bounded self-adjoint map on $L^2(D, \mathbb{R}^d)$ with $\nabla H_0^1(D)$, $H(\operatorname{div} 0, D)$ and W as invariant subspaces. On $\nabla H_0^1(\Omega)$, $N_D^0[\phi] = \phi$, on $H(\operatorname{div} 0, D)$, $N_D^0[\phi] = 0$ and on W:

$$\nu \cdot N_D^0[\phi] = \left(\frac{1}{2} + \mathcal{K}_D^*\right) [\phi \cdot \nu] \text{ on } \partial D,$$

where ν is the outward normal on ∂D and $K_D^*: L^2(\partial D) \to L^2(\partial D)$ is the Neumann-Poincaré operator associated with ∂D . Moreover, $N_D^0|_W: W \longrightarrow W$ is a compact operator and hence, the spectrum of $N_D^0|_W$ is discrete and the associated eigenfunctions form a basis of W.

We refer the reader to [3] for the properties of the Neumann-Poincaré operator. Therefore, using Lemma 3.3, we have

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

So, since

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

see [5] and [6, Lemma 4.2], the term $L^{-1}\widetilde{R}[v]$ can be neglected, and the following asymptotic expansion holds:

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

Moreover, from [6, Proposition 3.1] (see also Appendix C), it follows that

$$(L^{-1}[\nabla e_{j_0}], \nabla e_{j_0}) \simeq \delta^d M(\mu_m/\mu_c, B) \nabla e_{j_0}(z; \omega_0) \cdot \nabla e_{j_0}(z; \omega_0), \tag{9}$$

where M is the polarization tensor given by [4]

$$M(\mu_m/\mu_c, B) = \left(\frac{\mu_m}{\mu_c} - 1\right) \int_{\partial B} \frac{\partial v^{(1)}}{\partial \nu} \Big|_{-}(\xi) \xi \, d\sigma(\xi),$$

with $v^{(1)}$ being such that

$$\begin{cases}
\Delta_{\xi} v^{(1)} = 0 & \text{in } \mathbb{R}^{d} \setminus \bar{B}, \\
\Delta_{\xi} v^{(1)} = 0 & \text{in } B, \\
\frac{\partial v^{(1)}}{\partial \nu}|_{+} = (\mu_{m}/\mu_{c}) \frac{\partial v^{(1)}}{\partial \nu}|_{-} & \text{on } \partial B, \\
v^{(1)}(\xi) \sim \xi & \text{as } |\xi| \to +\infty.
\end{cases} \tag{10}$$

The proof is then complete.

4 Shift of the scattering resonances by external small particles

Now consider the case where the particle is outside Ω . The main difference in this case is that the modes of K_{Ω}^{ω} are not defined on D, and therefore we must first write the expansion for G outside of Ω . We start by recalling the Lippmann-Schwinger equation for $v = G - \Gamma_m$:

$$\left(I - \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega}\right) \left[v(\cdot, x_0)\right](x) = \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega} \left[\Gamma_m(\cdot, x_0)\right](x) \qquad \text{for } x, x_0 \in \Omega.$$

Now, using Proposition 2.10 for z and z' inside Ω we have

$$v(z, z'; \omega) = c_{j_0}(\omega) \frac{e_{j_0}(z; \omega) e_{j_0}(z'; \omega)}{\omega - \omega_0} + \widetilde{R}(z, z'; \omega),$$

and we can write an expansion for $v(x, x_0)$ for $x \in \mathbb{R}^d \setminus \Omega$:

$$v(x,x_0) - \frac{\omega^2 \tau \varepsilon_c \mu_m c_{j_0}(\omega)}{\omega - \omega_0} \int_{\Omega} e_{j_0}(z,\omega) \Gamma_m(z,x) e_{j_0}(x_0,\omega) dz - \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega} [\widetilde{R}(\cdot,x_0;\omega)](x)$$

$$= \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega} [\Gamma_m(\cdot,x_0)](x) \qquad x \in \mathbb{R}^d, x_0 \in \Omega$$

The latter equality can be written as

$$v(x,x_0) = \frac{\omega^2 \tau \varepsilon_c \mu_m c_{j_0}(\omega)}{\omega - \omega_0} \left(\int_{\Omega} e_{j_0}(z,\omega) \Gamma_m(z,x) dz \right) e_{j_0}(x_0,\omega) + R_1(x,x_0,\omega), \qquad x \in \mathbb{R}^d, x_0 \in \Omega.$$

where R_1 is regular in space and holomorphic in ω . Let

$$g_{j_0}(x;\omega) := \omega^2 \tau \varepsilon_c \mu_m \int_{\Omega} e_{j_0}(z';\omega) \Gamma_m(z,x;\omega) dz', \qquad x \in \mathbb{R}^d.$$

We have

$$v(x, x_0) = \frac{c_{j_0}(\omega)}{\omega - \omega_0} g_{j_0}(x; \omega) e_{j_0}(x_0, \omega) + R_1(x, x_0, \omega), \qquad x \in \mathbb{R}^d, x_0 \in \Omega.$$

We can now use this expansion in the Lippmann-Schwinger equation again:

$$v(x,x_0) - \frac{\omega^2 \tau \varepsilon_c \mu_m c_{j_0}(\omega)}{\omega - \omega_0} g_{j_0}(x;\omega) \left(\int_{\Omega} e_{j_0}(z,\omega) \Gamma_m(z,x_0) dz \right) - \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega} [R_1(\cdot,x_0,\omega)](x)$$

$$= \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega} [\Gamma_m(\cdot,x_0)](x) \qquad x \in \mathbb{R}^d, x_0 \in \mathbb{R}^d.$$

Therefore, we have an expansion for v outside of Ω :

$$v(x, x_0) = \frac{c_{j_0}(\omega)}{\omega - \omega_0} g_{j_0}(x; \omega) g_{j_0}(x_0; \omega) + R_2(x, x_0, \omega), \qquad x \in \mathbb{R}^d, x_0 \in \mathbb{R}^d.$$

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 a neighborhood $V(\omega_0)$ of ω_0 . Therefore, by exactly the same method as in the previous section, the following asymptotic expansion can be obtained.

Proposition 4.1. As $\delta \to 0$, we have

$$\omega_{\delta} - \omega_0 \simeq \delta^d c_{i_0}(\omega_0) M(\mu_m/\mu_c, B) \nabla g_{i_0}(z; \omega_0) \cdot \nabla g_{i_0}(z; \omega_0). \tag{11}$$

5 Shift of the scattering resonances due to resonant particles

Let $D \in \Omega$ and suppose that D is such that μ_c depends on ω and for a discrete set of frequencies ω , that we can call subwavelength resonances, problem (10) (or equivalently the operator $\left(\frac{\mu_m + \mu_c}{2(\mu_m - \mu_c)}I - K_D^*\right)^{-1}$) is nearly singular, see [2, 7, 8]. In that case, we have the following scattering resonance problem: Find ω such that there is a non-trivial solution v to

$$L(\omega)[v] - \frac{c_{j_0}(\omega)}{\omega - \omega_0}(v, \nabla e_{j_0})\nabla e_{j_0} + R[v] = 0,$$
(12)

where $L(\omega)$ is defined by (8). Using, for instance, the Drude model for μ_c , we have $\mu_c(\omega) = \mu_m(1 - \omega_p^2/\omega^2)$, where ω_p is a given frequency.

It is easy to see that the nearly singular character of (10) is linked to the non-invertibilty of $L(\omega)$ on W.

Denote by $P_1: L^2(D, \mathbb{R}^d) \longrightarrow L^2(D, \mathbb{R}^d)$ the orthogonal projector on $\nabla H_0^1(D)$ and $P_2: L^2(D, \mathbb{R}^d) \longrightarrow L^2(D, \mathbb{R}^d)$ the orthogonal projector on H(div 0, D). Using Lemma 3.3, we can write the resolvent operator $L^{-1}(\omega)$ as follows:

$$L(\omega)^{-1} = \frac{1}{1 - \lambda(\omega)} P_1 + \frac{1}{\lambda(\omega)} P_2 + \sum_{i} \frac{(\cdot, \varphi_i) \varphi_j}{\lambda(\omega) - \lambda_j},$$

where $(\lambda_j, \varphi_j)_j$ are the pairs of eigenvalues and associated orthonormal eigenfunctions of N_D^0 . We can then rewrite equation (12) as follows:

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

Now, taking the scalar product on $L^2(D, \mathbb{R}^d)$ with ∇e_{j_0} and multiplying by $(\omega - \omega_0)(\lambda(\omega) - \lambda_j)$, we obtain that

$$(\omega - \omega_0)(\lambda(\omega) - \lambda_j)(v, \nabla e_{j_0}) - c_{j_0}(\omega_0)(v, \nabla e_{j_0})(\nabla e_{j_0}, \varphi_j)^2 + (\omega - \omega_0)(\lambda(\omega) - \lambda_j)L^{-1}R[v] = 0.$$

Since R is analytic in ω , the remainder $(\omega - \omega_0)(\lambda(\omega) - \lambda_j)L^{-1}R[v]$ is negligible in a neighborhood of ω_0 . Hence, we arrive at the following proposition:

Proposition 5.1. As $\delta \to 0$, we have

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

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

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

Hence, we have a significant shift in the scattering resonances if the particle D is resonant near or at the frequency ω_0 . In fact, the shift in the scattering resonance is proportional to the square root of the particle's volume. This anomalous effect has been observed in [19].

6 Asymptotic analysis near exceptional scattering resonances

In this section, we consider the asymptotic behavior of an exceptional scattering resonance for a particular form of the Green's function. These exceptional resonances are due to the non-Hermitian character of the operator T_D^{ω} , see [9,18]. For simplicity and in view of the Jordan-type decomposition of the operator T_D^{ω} established in [9], we assume that, for ω near ω_0 , $G(x, y; \omega)$ behaves like

$$G(x,y;\omega) = \Gamma_m(x,y;\omega) + c_1(\omega) \frac{h^{(1)}(x;\omega)h^{(1)}(y;\omega)}{\omega - \omega_0} + c_2(\omega) \frac{h^{(2)}(x;\omega)h^{(2)}(y;\omega)}{(\omega - \omega_0)^2} + R(x,y;\omega), (13)$$

for two functions $h^{(1)}$ and $h^{(2)}$ in $L^2(D)$. Here, the functions $\omega \mapsto c_j(\omega)$, j = 1, 2 and $\omega \mapsto R(x, y; \omega)$ are all analytic in a neighborhood of ω_0 , and $(x, y) \mapsto R(x, y; \omega)$ is smooth.

In this simple case, where the exceptional scattering resonance is of second-order, we characterize the splitting of the scattering resonance ω_0 due to the small particle D, which is assumed for simplicity to be non-resonant.

Following the same arguments as those in the previous sections, we neglect R in (13) and 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 equations by $\nabla h^{(1)}$ and $\nabla h^{(2)}$, respectively, and integrating by parts over D, we obtain the following system of equations:

$$\begin{cases} (v, \nabla h^{(1)}) \left(1 - c_1(\omega) \frac{(L^{-1}[\nabla h^{(1)}], \nabla h^{(1)})}{\omega - \omega_0} \right) = c_2(\omega)(v, \nabla h^{(2)}) \frac{(L^{-1}[\nabla h^{(2)}], \nabla h^{(1)})}{(\omega - \omega_0)^2}, \\ (v, \nabla h^{(2)}) \left(1 - c_2(\omega) \frac{(L^{-1}[\nabla h^{(2)}], \nabla h^{(2)})}{(\omega - \omega_0)^2} \right) = c_1(\omega)(v, \nabla h^{(1)}) \frac{(L^{-1}[\nabla h^{(1)}], \nabla h^{(2)})}{\omega - \omega_0}. \end{cases}$$

Therefore, the following result holds.

Proposition 6.1. Assume that the decomposition (13) holds for ω near ω_0 . Then the perturbed scattering resonance problem (due to the particle D) can be approximately reformulated as a search for ω near ω_0 such that the matrix

$$\mathcal{A}(\omega) := \begin{pmatrix} 1 - c_1(\omega) \frac{(L^{-1}[\nabla h^{(1)}], \nabla h^{(1)})}{\omega - \omega_0} & -c_2(\omega) \frac{(L^{-1}[\nabla h^{(2)}], \nabla h^{(1)})}{(\omega - \omega_0)^2} \\ c_1(\omega) \frac{(L^{-1}[\nabla h^{(1)}], \nabla h^{(2)})}{\omega - \omega_0} & 1 - c_2(\omega) \frac{(L^{-1}[\nabla h^{(2)}], \nabla h^{(2)})}{(\omega - \omega_0)^2} \end{pmatrix}$$

is singular.

In view of Proposition 6.1, the second-order exceptional scattering frequency is split into two scattering frequencies which can be computed approximately by finding the values of ω for which the determinant of the matrix $\mathcal{A}(\omega)$ is zero.

Assume that $(L^{-1}[\nabla h^{(1)}], \nabla h^{(2)}) = 0$. Then, it can be easily seen that the splitting of ω_0 is of order the square root of the volume of the particle. This is in contrast with (6), where the perturbation induced by the small particle is proportional to its volume.

It is worth emphasizing that the derivations presented in this section can be generalized to the case of exceptional points of arbitrary order N. In this case, it is expected that the splitting induced by a small particle on an exceptional scattering frequency of order N is proportional to the volume of the particle to the power 1/N.

7 Concluding remarks

In this paper, the leading-order term in the shifts of scattering resonances of a radiating dielectric cavity due to the presence of small particles is derived. The formula describes the dependency of the frequency shifts on the position and the polarization tensor of the particle. It is also proved that the shift is significantly enhanced if the particle is a subwavelength resonant particle and resonates near or at a scattering resonance of the cavity. A characterization of the splitting of the scattering resonances due to small particles near an exceptional scattering resonance is performed. It would be challenging to develop a general theory near such frequencies. This would be the subject of a forthcoming paper.

A Proof of Proposition 2.10

Proof. The proof follows an idea from [9]. Denote by v the difference

$$v(x,y) = G(x,y,\omega) - \Gamma_m(x,y,\omega).$$

One can check that $v(\cdot, x_0)$ is a solution of the following integral equation:

$$(I - \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega}) [v] = \omega^2 \tau \varepsilon_c \mu_m K_{\Omega}^{\omega} [\Gamma_m(\cdot, x_0)].$$

Therefore,

$$v = \left(\frac{1}{\omega^2 \tau \varepsilon_c \mu_m} I - K_{\Omega}^{\omega}\right)^{-1} K_{\Omega}^{\omega} \left[\Gamma_m(\cdot, x_0)\right].$$

Under the assumption that ω_0 is a non exceptional scattering resonance (see Definition 2.8) we can perform a pole pencil decomposition of the resolvent of K_{Ω}^{ω} . We start from the spectral decomposition of the compact operator K_{Ω}^{ω} on $L^2(\Omega)$. The eigenspace associated with the eigenvalue $\frac{1}{\omega_0^2 \tau \varepsilon_c \mu_m}$ is of dimension one, and we denote by e_{j_0} its basis. One can then write

$$\left(\frac{1}{\omega^2 \tau \varepsilon_c \mu_m} - K_{\Omega}^{\omega}\right)^{-1} = \frac{1}{\left(\omega^2 \tau \varepsilon_c \mu_m\right)^{-1} - \lambda_{j_0}(\omega_0)} (e_{j_0}, \cdot) e_{j_0} + \hat{R}(\cdot, \omega),$$

where (,) denotes the L^2 real scalar product on Ω , and $\omega \mapsto \hat{R}(\cdot, \omega) \in L^2(\Omega)$ is analytic in a complex neighborhood V of ω_0 . Using

$$1 - \omega^2 \tau \varepsilon_c \mu_m \lambda_{i_0}(\omega) = R(\omega)(\omega - \omega_0)$$

and composing with K_{Ω}^{ω} , we obtain that

$$v(x,x_0) = \widetilde{c}_{j_0}(\omega) \frac{1}{\omega - \omega_0} (e_{j_0}, K_{\Omega}^{\omega} \left[\Gamma_m(\cdot, x_0) \right]) e_{j_0}(x) + \widetilde{R}(x,x_0;\omega).$$

Now we note that

$$\Gamma_m(x,y) = -K_{\Omega}^{\omega} \left[\delta(\cdot - y) \right](x) \text{ for all } x, y \in \mathbb{R}^d, x \neq y.$$

Using the completeness relation given in Lemma 2.7 yields

$$\Gamma_m(x,y) = \sum_j \lambda_j(\omega) e_j(y) e_j(x),$$

for some constants λ_i . Now, we can write that

$$(e_{j_0}, K_{\Omega}^{\omega}[\Gamma_m(\cdot, x_0)]) = e_j(x_0)(e_{j_0}, \lambda_{j_0}(\omega)e_{j_0}),$$

to arrive at

$$v(x,x_0) = c_{j_0}(\omega) \frac{1}{\omega - \omega_0} e_{j_0}(x_0) e_{j_0}(x) + \widetilde{R}(x,x_0;\omega).$$

B Proof of Lemma 3.2

Proof. The operator T_D is a singular integral operator of the Calderón-Zygmund type, see [11]. This type of singular operator often arises in electrostatic and magnetostatic theories (see the appendix of [6] for a simple review of the properties of these operators within the formalism of Green's functions) The fact that T_D^{ω} is well defined can be deduced directly from Proposition 2.10. Since G can be written as $G(x,y) = \Gamma_m(x,y) + K(x,y)$ where K is a smooth kernel, we can see that the singularity of the derivatives of G is the same as that of the derivatives of Γ_m , that is $\partial_{x_i,x_j}G(x,y) = \partial_{x_i,x_j}\Gamma_m(x,y) + K_{i,j}(x,y)$. Therefore, it is easy to see that the singular part of $\partial_{x_i,x_j}G(x,y)$ satisfies the same cancellation property as $\partial_{x_i,x_j}\Gamma_m(x,y)$, that is,

$$\int_{x+\mathbb{S}^{d-1}} \partial_{x_i,x_j} \Gamma_m(x,y) dy = 0.$$

Hence, the fact that T_D is defined on $L^2(D, \mathbb{R}^d)$ follows directly from classical Calderón-Zygmund theory and the cancellation property above.

C Proof of estimate (9)

Here, we give some more details on how to obtain (9) from the results of [6].

Lemma C.1. As $\delta \to 0$, we have

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

Proof. From [6, Proposition 3.1], one can see that if φ satisfies

$$\begin{cases} \nabla \cdot \left(\frac{1}{\mu} \nabla \varphi\right) = 0 & \text{in } \mathbb{R}^d, \\ \nabla \varphi(x) - e_{j_0} = O\left(|x|^{-d+1}\right) & \text{as } |x| \to +\infty. \end{cases}$$

then $\nabla \varphi$ solves the integral equation

$$\left(\frac{1}{\mu_m}I - \left(\frac{1}{\mu_c} - \frac{1}{\mu_m}\right)N_D^0\right)[\nabla\varphi] = \frac{1}{\mu_m}\nabla e_{j_0},$$

which is exactly

$$L[\varphi] = \nabla e_{j_0}.$$

Now, replacing ∇e_{j_0} by its average and controlling the reminder via the Cauchy-Schwartz inequality we have:

$$(L^{-1}[\nabla e_{j_0}], \nabla e_{j_0}) = (L^{-1}[\nabla e_{j_0}], \frac{1}{|D|} \int_D \nabla e_{j_0}) + (L^{-1}[\nabla e_{j_0}], \nabla e_{j_0} - \frac{1}{|D|} \int_D \nabla e_{j_0})$$

$$= \frac{1}{|D|} \int_D L^{-1}[\nabla e_{j_0}] \cdot \int_D \nabla e_{j_0} + O\left(\delta^2\right).$$

But the average of $\nabla \varphi$ is exactly the dipole moment, which is given by the polarization tensor applied to the average of the exciting field:

$$\int_{D} L^{-1}[\nabla e_{j_0}] = M(\mu_m/\mu_c, D) \int_{D} \nabla e_{j_0} = \delta^d M(\mu_m/\mu_c, B).$$

Since $\frac{1}{|D|} \int_D \nabla e_{j_0}(x) dx - \nabla e_{j_0}(z) = O(\delta)$ (recall that e_j is a mode of the cavity, and is therefore independent of δ) we can replace the average of ∇e_{j_0} by its value at the center of D to get the result.

References

- [1] H. Ammari, A. Dabrowski, B. Fitzpatrick, and P. Millien, Perturbations of the scattering resonances of an open cavity by small particles. Part I: The transverse magnetic polarization case, submitted.
- [2] H. Ammari, Y. Deng, and P. Millien, Surface plasmon resonance of nanoparticles and applications in imaging, Arch. Ration. Mech. Anal., 220 (2016), 109–153.
- [3] H. Ammari, B. Fitzpatrick, H. Kang, M. Ruiz, S. Yu, and H. Zhang, *Mathematical and computational methods in photonics and phononics*, Mathematical Surveys and Monographs, Vol. 235, American Mathematical Society, Providence, 2018.
- [4] H. Ammari and H. Kang, Polarization and moment tensors. With applications to inverse problems and effective medium theory, Applied Mathematical Sciences, 162. Springer, New York, 2007.
- [5] H. Ammari, H. Kang, and H. Lee, Layer potential techniques in spectral analysis, Mathematical Surveys and Monographs, 153, American Mathematical Society, Providence, RI, 2009.
- [6] H. Ammari and P. Millien, Shape and size dependence of dipolar plasmonic resonance of nanoparticles, J. Math. Pures Appl., DOI: https://doi.org/10.1016/j.matpur.2018.12.001 (arXiv:1804.11092).
- [7] H. Ammari, P. Millien, M. Ruiz, and H. Zhang, Mathematical analysis of plasmonic nanoparticles: the scalar case, Arch. Ration. Mech. Anal., 224 (2017), 597–658.
- [8] H. Ammari, M. Ruiz, S. Yu, and H. Zhang, Mathematical analysis of plasmonic resonances for nanoparticles: the full Maxwell equations, J. Differential Equations 261 (2016), 3615–3669.
- [9] H. Ammari and H. Zhang, Super-resolution in high-contrast media, Proc. A. 471 (2015), 20140946, 11 pp.
- [10] M. Aspelmeyer, T.J. Kippenberg, and F. Marquardt, Cavity optomechanics, Rev. Modern Phys., 86 (2014), 1392–1452.
- [11] A.P. Calderón and A. Zygmund, On the existence of certain singular integrals, Acta Mathematica, 88 (1952), 85–139.
- [12] H. Cao and J. Wiersig, Dielectric microcavities: Model systems for wave chaos and non-Hermitian physics, Rev. Modern Phys., 87 (2015), 61–111.
- [13] W. Chen, S.K. Özdemir, G. Zhao, J. Wiersig, and L. Yang, Exceptional points enhance sensing in an optical microcavity, Nature, 548 (2017), 192–196.

- [14] M. Costabel, E. Darrigrand, and H. Sakly, The essential spectrum of the volume integral operator in electromagnetic scattering by a homogeneous body, Comptes Rendus Math., 350 (2012), 193–197.
- [15] M.J. Friedman and J.E. Pasciak, Spectral properties for the magnetization integral operator, Math. Comp., 43 (1984), 447–453.
- [16] W.D. Heiss, The physics of exceptional points, J. Phys. A: Math. Theor., 45 (2012), 444016 (11p).
- [17] M.-A. Miri and Andrea Alù, Exceptional points in optics and photonics, Science, 363 (2019), eaar7709.
- [18] A. Pick, B. Zhen, O.D. Miller, C.W. Hsu, F. Hernandez, A.W. Rodriguez, M. Soljacic, and S.G. Johnson, General theory of spontaneous emission near exceptional points, Optics Express, 25 (2017), 290505.
- [19] F. Ruesink, H.M. Doeleman, R. Hendrikx, A.F. Koenderink, and E. Verhagen, Perturbing open cavities: Anomalous resonance frequency shifts in a hybrid cavity-nanoantenna system, Phys. Rev. Lett., 115 (2015), 203904.
- [20] M.A. Schmidt, D. Yuan Lei, L. Wondraczek, V. Nazaba, and S.A. Maier, Hybrid nanoparticle-microcavity-based plasmonic nanosensors with improved detection resolution and extended remote-sensing ability, Nature Communications, 1108 (2012), 2019.