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Perturbation of the scattering resonances of an open cavity by small particles. Part I: The transverse magnetic polarization case

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Abstract

This paper aims at providing a small-volume expansion framework for the scattering resonances of an open cavity perturbed by small particles. The shift of the scattering frequencies induced by the small particles is derived without neglecting the radiation effect. The formula holds for arbitrary-shaped particles. It shows a strong enhancement in the frequency shift in the case of subwavelength particles with dipole resonances. The formula is 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 presented.

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

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1 Introduction

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 [22, 36, 43]. Open optical cavities are used to detect, characterize, and determine the size of small particles. They show great promise for a broad range of physical sensing applications that rely on sensitive detection of resonance shifts to probe internal or external physical parameter changes [48]. Sensitive detection of small particles is essential for a variety of applications ranging from medical diagnostics and drug discovery to security screening and environmental science, amongst others. The binding of a small particle to an open optical cavity perturbs the cavity mode at a resonance wavelength resulting in a cavity

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resonance shift. The Bethe-Schwinger closed cavity perturbation formula [16] (see also [13] for its rigorous derivation) has been widely employed in the case of radiating cavities in order to characterize the properties of the small particle from the induced cavity resonance shifts. Unfortunately, this formula omits the radiation effect (see, for instance, [20]). Moreover, since it is established only for spherical particles, it can not be used to retrieve the orientation of the particle. Note that the detection of the particle's orientation is of great concern in bio-sensing [38]. In this paper, we 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. The small-volume asymptotic formula in this paper generalizes to the open cavity case those derived in [5, 6, 9, 13]. 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.

For simplicity, we consider the transverse magnetic polarization case. For the analysis of the transverse electric case we refer the reader to [1]. Transverse magnetic and electric polarizations can be excited separately in some open cavities and the shifts in the resonances can be measured efficiently [27, 38]. The case of the full Maxwell equations can be treated by the same approach developed here. Two cases are considered in this paper: the one-dimensional case and the multi-dimensional case. The applicability of our approach to the perturbations of whispering-gallery modes by external arbitrary-shaped particles is also discussed. Whispering-gallery modes are a subclass of resonances which are characterized by their surface mode nature [20]. They can occur in optical cavities possessing a closed concave surface. Spherical, disc, and ring cavities represent the simplest resonator geometry and have then seen much attention in the literature over the years [20]. Their resonant shifts are used to image particles near the surface of the optical cavity. Finally, we characterize the effect that an arbitrary shaped subwavelength particle, which is bound to the surface of the cavity, has on the whispering-gallery modes of the cavity due to the particle's dipole resonances. The coupling between the subwavelength resonant particle and the cavity modes is essential for imaging the particle. In fact, as proved in this paper, since the shift of the scattering frequencies is proportional to the polarization of the particle [2, 7, 8, 11], which blows-up at subwavelength resonances, the effect of a subwavelength resonant particle on the cavity modes can be significant. 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. It is worth emphasizing that the existence of exceptional scattering resonances is due to the non-hermitian character of the scattering resonance problem. For the analysis of exceptional points, we again refer the reader to [1]. The analysis of such a challenging problem is much simpler in the transverse electric case than in the transverse magnetic one. The reader is also referred to [23–25] for small amplitude sensitivity analyses of the scattering resonances. Numerical computation of resonances has been addressed, for instance, in [21, 26, 31, 32, 40, 47].

The paper is organized as follows. In Section 2, 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 3 generalizes the method to the multi-dimensional case. In Section 4, we consider the perturbation of whispering-gallery modes by small particles. A formula is obtained for the shifting of the frequencies and it shows that there is a strong enhancement in the frequency shifts in the case of subwavelength resonant 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 5, we present some numerical examples to illustrate the accuracy of the formulas derived in this paper and their use in the sensing of small particles. The paper ends with some concluding remarks.

2 One dimensional case

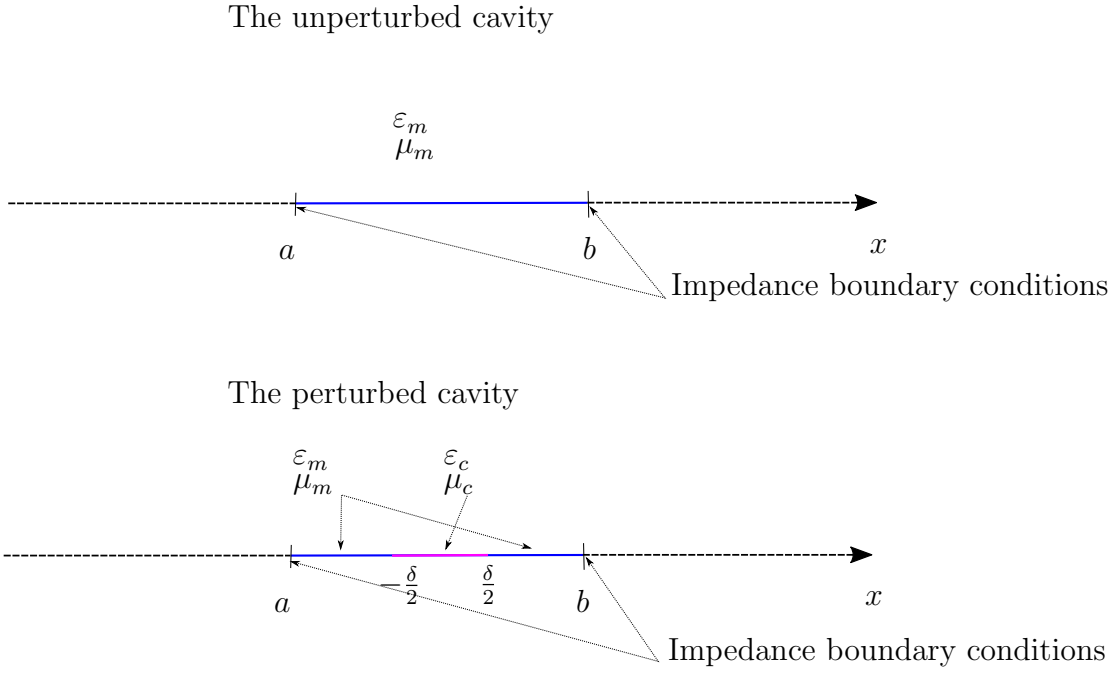


Figure 1: One dimensional cavity.

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 $(-\delta/2, \delta/2)$, see Figure 1. Here, $a < b$, $\delta > 0$ is small, 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,

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

We now consider the perturbed problem: we seek a solution u_δ , for which $\omega_\delta \rightarrow \omega_0$ as

$\delta \rightarrow 0$ of the following equation:

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

Remark 2.1. 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 [24]. 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, we must go to the time domain, see, for instance, [21, 24].

Proposition 2.2. *As $\delta \rightarrow 0$, we have*

$$\omega_\delta = \omega_0 + \delta\omega_1 + O(\delta^2),$$

where

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

The polarization α is defined by

$$\alpha = \left(\frac{\varepsilon_m}{\varepsilon_c} - 1 \right) \partial_x v^{(1)}\left(\frac{1}{2}\right)|_-, \quad (3)$$

and $v^{(1)}$ is the unique solution (up to a constant) of the auxiliary differential equation:

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

with $\tilde{\varepsilon} = \varepsilon_c \chi_{(-1/2, 1/2)} + \varepsilon_m \chi_{\mathbb{R} \setminus (-1/2, 1/2)}$. Here, $|_-$ indicates the limit at $(1/2)^-$ and χ_I denotes the characteristic function of the set I .

Remark 2.3. Note that the polarization α can be computed explicitly. It is given by $\alpha = 1 - (\varepsilon_c/\varepsilon_m)$.

Proof. Using the method of matched asymptotic expansions for δ small, see [6], 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 (1) and formally equate coefficients of δ^{-2} and δ^{-1} , then we obtain

$$\partial_\xi((1/\tilde{\varepsilon})\partial_\xi e_0) = 0,$$

and

$$\partial_\xi((1/\tilde{\varepsilon})\partial_\xi e_1) = 0,$$

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

$$e_1(\xi) \sim \xi \partial_x u_0(0) \quad \text{as } |\xi| \rightarrow +\infty. \quad (4)$$

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

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

Let $G(\xi) = |\xi|/2$ be the free space Green function,

$$\partial_\xi^2 G(\xi - \xi') = \delta_0(\xi - \xi').$$

Since

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

we have

$$v^{(1)}(\xi) = \xi + (1 - (\varepsilon_m/\varepsilon_c))\partial_\xi v^{(1)}(-1/2)|_+ G(\xi + 1/2) + ((\varepsilon_m/\varepsilon_c) - 1)\partial_\xi v^{(1)}(1/2)|_- G(\xi - 1/2),$$

where the subscripts $+$ and $-$ indicate the limits at $(1/2)^-$ and $(1/2)^+$, respectively. 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,

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

On the other hand,

$$G(\xi - 1/2) \sim |\xi| - \xi/(2|\xi|) + \dots,$$

and

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

Therefore,

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

Assume first that $\mu_m = \mu_c$. The second matching condition (4) yields

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

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 ρ small enough. Upon using the radiation condition and Green's theorem, as ρ goes to zero we obtain

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

where the polarization α is given by

$$\alpha = ((\varepsilon_m/\varepsilon_c) - 1)\partial_\xi v^{(1)}(1/2)|_- = 1 - \frac{\varepsilon_c}{\varepsilon_m}. \quad (5)$$

Therefore, we arrive at

$$\omega_1 = \frac{\alpha (\partial_x u_0(0))^2}{2\omega_0 \mu_m \varepsilon_m \int_a^b u_0^2 dx + i\varepsilon_m ((u_0(a))^2 + (u_0(b))^2)}. \quad (6)$$

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

Now, if $\mu_c \neq \mu_m$, then 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

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

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

$$\partial_x^2 u_0(0) = -\omega_0^2 \mu_m \varepsilon_m u_0(0). \quad (7)$$

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

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

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,

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

Then

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

and so

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

which yields the result. \blacksquare

Remark 2.4. Proposition 2.2 can be easily generalized to the case where ε_m and μ_m are variable in (a, b) . Under the normalization $\int_a^b \varepsilon_m(x)\mu_m(x)|u_0(x)|^2 dx = 1$, the shift in the scattering resonance ω_1 is given by

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

where the polarization α is defined by

$$\alpha = \left(\frac{\varepsilon_m(0)}{\varepsilon_c} - 1 \right) \partial_x v^{(1)}\left(\frac{1}{2}\right)\Big|_-,$$

and $v^{(1)}$ is the unique solution (up to a constant) of

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

with $\tilde{\varepsilon} = \varepsilon_c\chi_{(-1/2, 1/2)} + \varepsilon_m(0)\chi_{\mathbb{R}\setminus(-1/2, 1/2)}$. The term $\varepsilon_m(0)\partial_x(1/\varepsilon_m)(0)\partial_x u_0(0)u_0(0)$ comes from the fact that

$$\partial_x^2 u_0(0) = -\omega_0^2 \mu_m(0)\varepsilon_m(0)u_0(0) - \varepsilon_m(0)\partial_x(1/\varepsilon_m)(0)\partial_x u_0(0),$$

instead of (7).

3 Multi-dimensional case

In this section, we generalize (2) to the multi-dimensional case. In dimension two, the formula obtained corresponds, as in the one-dimensional case, to an open cavity with the transverse magnetic polarization [25]. We use the same notation as in Section 2.

Let Ω be a bounded domain in \mathbb{R}^d for $d = 2, 3$, with smooth boundary $\partial\Omega$, see Figure 2. Let ω_0 be a simple eigenvalue of the unperturbed open cavity. Then there exists a non trivial solution u_0 to the equation:

Cavity perturbed by an internal particle

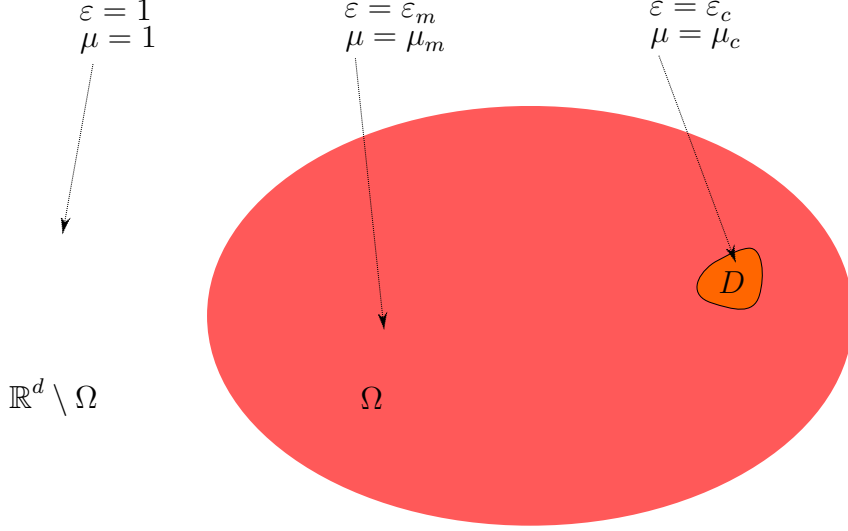


Figure 2: Multi-dimensional cavity.

$$\begin{cases} \nabla \cdot ((1/\varepsilon)\nabla u) + \omega_0^2 \mu u = 0 & \text{in } \mathbb{R}^d, \\ \varepsilon_m \mu_m \int_{\Omega} |u|^2 dx = 1, \\ u \text{ satisfies the outgoing radiation condition,} \end{cases} \quad (8)$$

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 . We refer to [21] for a precise statement of the outgoing radiation condition.

In order to express the radiation condition, we consider a ball large enough to contain the domain Ω . Here, 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 [10]

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

where

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

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).

Then the outgoing radiation condition is as follows:

$$(1/\varepsilon_m) \frac{\partial u_0}{\partial \nu} = T_{\omega_0}[u_0] \text{ on } \partial\Omega. \quad (9)$$

Note also that the above explicit version of the capacity operator will be used in Section 5 to test the validity of our formula. Then, (8) is equivalent to

$$\begin{cases} (1/\varepsilon_m) \Delta u_0 + \omega_0^2 \mu u_0 = 0 & \text{in } \Omega, \\ (1/\varepsilon_m) \frac{\partial u_0}{\partial \nu} = T_{\omega_0}[u_0] & \text{on } \partial\Omega, \\ \varepsilon_m \mu_m \int_{\Omega} |u_0|^2 = 1, \end{cases} \quad (10)$$

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 since on one hand, $z_{-m}(\omega, R) = z_m(\omega, R)$ for all $m \in \mathbb{Z}$, and on the other hand, $Y_m^{-l} = (-1)^l \bar{Y}_m^l$, we have

$$\int_{\partial\Omega} T_{\omega}[f]g \, d\sigma = \int_{\partial\Omega} fT_{\omega}[g] \, d\sigma \quad \text{for all } f, g \in H^{1/2}(\partial\Omega), \quad (11)$$

for $d = 2, 3$, where $H^s(\partial\Omega)$ is the standard Sobolev space of order s .

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 . In view of (9), the eigenvalue problem is to find ω_{δ} such that there is a non-trivial couple $(\omega_{\delta}, u_{\delta})$ satisfying

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

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

Proposition 3.1. *As $\delta \rightarrow 0$, we have*

$$\omega_{\delta} = \omega_0 + \delta^d \omega_1 + O(\delta^{d+1}),$$

where

$$\omega_1 = \frac{M(\varepsilon_m/\varepsilon_c, B) \nabla u_0(z) \cdot \nabla u_0(z) + \omega_0^2 |B| \varepsilon_m (\mu_c - \mu_m) (u_0(z))^2}{2\omega_0 + \varepsilon_m \int_{\partial\Omega} \partial_{\omega} T_{\omega}|_{\omega=\omega_0}[u_0] u_0 \, d\sigma}, \quad (12)$$

with M being the polarization tensor associated with the domain B and $\varepsilon_m/\varepsilon_c$ the contrast defined by (15) with $v^{(1)}$ being given by (14).

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

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

where $\xi = (x-z)/\delta$. Therefore, 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

$$\begin{cases} ((1/\varepsilon_m)\Delta + \lambda_0 \mu_m)u_1(y) = -\lambda_1 \mu_m u_0(y) & \text{for } |y-z| \gg O(\delta), \\ (1/\varepsilon_m) \frac{\partial u_1}{\partial \nu} = T_{\omega_0}[u_1] + \omega_1 \partial_\omega T_\omega|_{\omega=\omega_0}[u_0] & \text{on } \partial\Omega, \end{cases} \quad (13)$$

and

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

for $j = 1, 2$. Imposing the matching conditions

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

and $y \rightarrow z$, we arrive at $e_0(\xi) \rightarrow u_0(z)$ 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 [6])

$$\begin{cases} \Delta_\xi v^{(1)} = 0 & \text{in } \mathbb{R}^d \setminus \bar{B}, \\ \Delta_\xi v^{(1)} = 0 & \text{in } B, \\ \frac{\partial v^{(1)}}{\partial \nu}|_+ = (\varepsilon_m/\varepsilon_c) \frac{\partial v^{(1)}}{\partial \nu}|_- & \text{on } \partial B, \\ v^{(1)}(\xi) \sim \xi & \text{as } |\xi| \rightarrow +\infty. \end{cases} \quad (14)$$

Let Γ be the fundamental solution of the Laplacian in \mathbb{R}^d . Let $M(\varepsilon_m/\varepsilon_c, B)$ be the polarization tensor associated with the domain B and the contrast $\varepsilon_m/\varepsilon_c$ given by [4]

$$M(\varepsilon_m/\varepsilon_c, B) = \left(\frac{\varepsilon_m}{\varepsilon_c} - 1\right) \int_{\partial B} \frac{\partial v^{(1)}}{\partial \nu}|_-(\xi) \xi \, d\sigma(\xi). \quad (15)$$

We refer the reader to [4] for the symmetry, positivity, and monotonicity of M . Then, by the same arguments as in [6, Section 4.1], it follows that

$$u_1(y) \sim -M(\varepsilon_m/\varepsilon_c, B) \nabla \Gamma(y-z) \cdot \nabla u_0(z) \quad \text{as } y \rightarrow z. \quad (16)$$

Multiplying (13) by u_0 and integrating by parts over $\Omega \setminus \bar{B}_\delta$, we obtain from (11) that

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

From (16), we have

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

Therefore,

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

and finally, we arrive at

$$\lambda_1 = \frac{M(\varepsilon_m/\varepsilon_c, B) \nabla u_0(z) \cdot \nabla u_0(z)}{1 + (1/(2\omega_0)) \varepsilon_m \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 d\sigma}, \quad (17)$$

or equivalently,

$$\omega_1 = \frac{M(\varepsilon_m/\varepsilon_c, B) \nabla u_0(z) \cdot \nabla u_0(z)}{2\omega_0 + \varepsilon_m \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 d\sigma}. \quad (18)$$

In the multi-dimensional case, the effect of radiation on the shift of the scattering resonance ω_0 is given by $\varepsilon_m \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 d\sigma$. Note also that formula (18) reduces to (6) in the one-dimensional case. In fact, the polarization tensor M reduces to α defined by (5) and the operator T_ω corresponds to multiplication by $-i\omega$ at a and $+i\omega$ at b . If one relaxes the assumption $\mu_c = \mu_m$, one can easily generalize formula (18) by computing, as in [6] and in Section 2, the second-order corrector e_2 . We then get the desired result. ■

4 Perturbations of whispering-gallery modes by an external particle

Whispering-gallery modes are modes which are confined near the boundary of the cavity. Their existence can be proved analytically or by a boundary layer approach based on WKB (high frequency) asymptotics [20, 30, 33, 35, 36, 39, 42]. Whispering-gallery modes are exploited to probe the local surroundings [28, 29, 37]. 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 [14, 20, 45, 46]. 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 $\Omega_\rho \setminus \bar{\Omega}$, see Figure 3. If

Cavity perturbed by an external particle

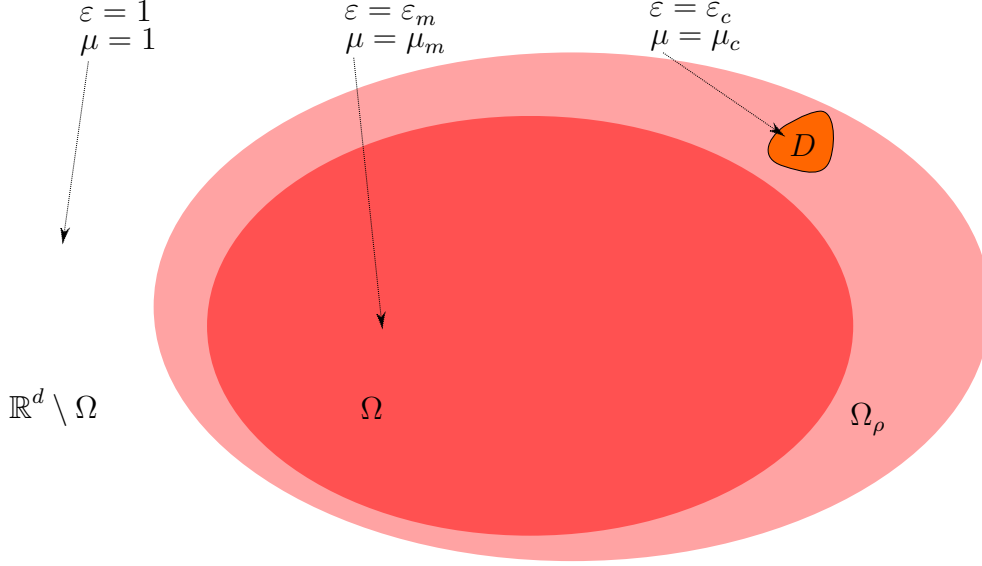


Figure 3: Perturbed cavity by an external particle.

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

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

Here, the polarization tensor $M(\varepsilon_m/\varepsilon_c, B)$ in (17) 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

$$v_0(x) = -\omega_0^2(\mu_m - 1) \int_{\Omega} \Gamma(x-y; \omega_0)u_0(y) dy + \left(\frac{1}{\varepsilon_m} - 1\right) \int_{\Omega} \nabla_y \Gamma(x-y; \omega_0) \cdot \nabla u_0(y) dy, \quad (19)$$

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 in order that the gradient of v_0 at the location of the particle has a significant magnitude.

Now, assume that the particle D is a subwavelength particle with dipole resonances, 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 subwavelength resonant frequencies, such that at these frequencies problem (14) is nearly singular, and therefore the polarization tensor associated with the particle D blows up, see [2, 8, 11]. Assume that the subwavelength resonant particle is coupled to the cavity, i.e., there is a whispering-gallery cavity mode ω_0 such that $\Re\omega_0$ is a subwavelength 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 the following proposition.

Proposition 4.1. *We have*

$$\omega_1 \simeq \frac{M((1/\varepsilon_c)(\Re\omega_0), B)\nabla v_0(z) \cdot \nabla v_0(z) + \omega_0^2|B|(\mu_c - 1)(v_0(z))^2}{2\omega_0 + \varepsilon_m \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 d\sigma}, \quad (20)$$

where v_0 is defined by (19).

Proposition 4.1 shows that despite their small size, subwavelength particles with dipole resonances significantly change the cavity modes when their subwavelength resonances are close to the cavity modes.

Finally, suppose that ω_0 is of multiplicity m . Then, following [12, 18, 19], ω_0 can be split into m scattering resonances $\omega_{\delta,j}$ having the following approximations:

$$\omega_{\delta,j}^2 \simeq \omega_0^2 + \delta^d \eta_j, \quad (21)$$

with η_j being the j -th eigenvalue of the matrix

$$\left(\frac{M\nabla v_{0,p}(z) \cdot \nabla v_{0,q}(z) + \omega_0^2|B|(\mu_c - 1)v_{0,p}(z)v_{0,q}(z)}{\mu_m \varepsilon_m \int_{\Omega} u_{0,p}u_{0,q} dx + (1/(2\omega_0)) \varepsilon_m \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_{0,q}]u_{0,p} d\sigma} \right)_{p,q=1}^m. \quad (22)$$

Here, $\{v_{0,q}\}_{q=1,\dots,m}$ are obtained by (19) with $\{u_{0,q}\}_{q=1,\dots,m}$ being an orthonormal eigenspace associated with ω_0 .

5 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 [34]. Our approach is as follows. We first use a projective eigensolver [15] 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 Muller's method [3].

It is well-known that boundary integral formulations of the exterior and transmission scattering problems are prone to so-called spurious resonances which can interfere with the search for the true scattering resonances [17]. In order to achieve a better separation between the spurious resonances and the true resonances when using the projective eigensolver, a combined field integral equation approach can be used [41, 44].

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 $\delta \rightarrow 0$ is plotted in Figure 4. Formula (21) matches the behavior of the eigenvalue perturbation as can be seen in Figure 5. On the other hand, we can easily reconstruct δ from a single scattering resonance shift.

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.

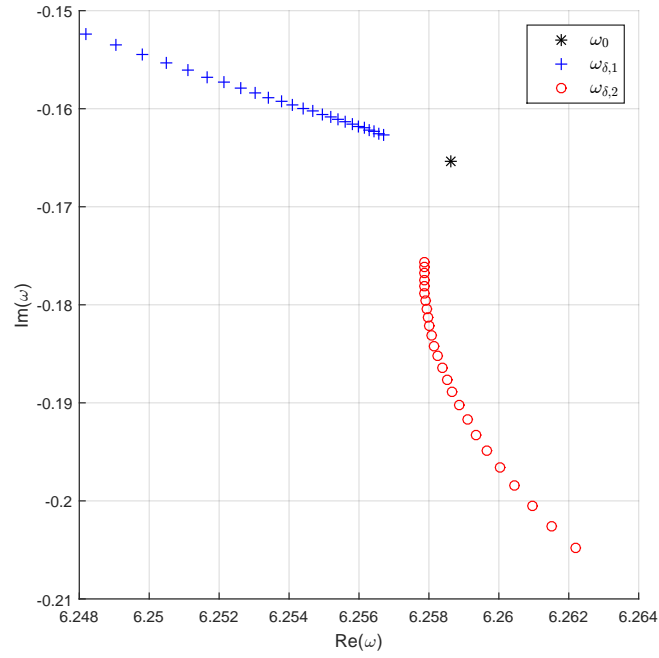


Figure 4: As the size of the small disk $\delta \rightarrow 0$, the perturbed whispering-gallery modes $\omega_{\delta,1}$ and $\omega_{\delta,2}$ converge towards the unperturbed mode ω_0 .

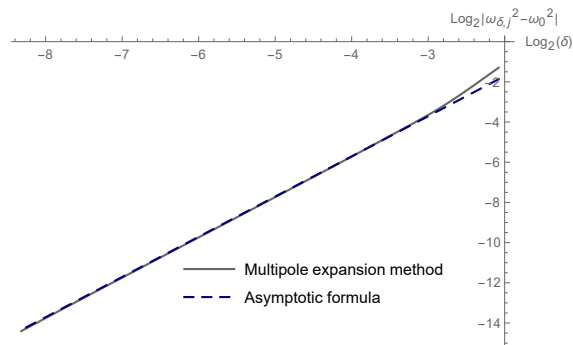


Figure 5: Comparison between the asymptotic formula for the perturbation $|\omega_{\delta,1}^2 - \omega_0^2|$ of the whispering-gallery mode and the perturbation computed numerically as the size of the small disk $\delta \rightarrow 0$.

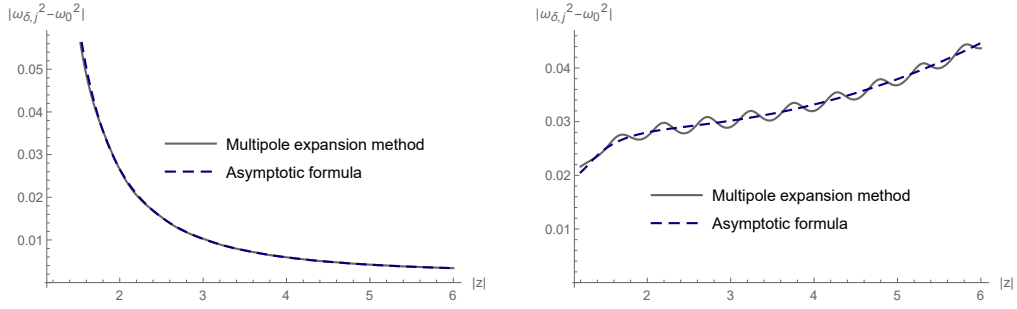


Figure 6: Comparison between the asymptotic formula for the perturbation $|\omega_{\delta,j}^2 - \omega_0^2|$ of the whispering-gallery mode and the perturbation computed numerically as the position of the inclusion $(z, 0)$ varies. The plot on the left corresponds to the perturbed resonance $\omega_{\delta,1}$ and the plot on the right corresponds to the perturbed resonance $\omega_{\delta,2}$.

By using (21), one can also reconstruct the polarization tensor. We highlight here the case of subwavelength resonant 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 $|\omega_{\delta,1}^2 - \omega_0^2|$ as $1/\varepsilon_c$ varies is presented in Figure 7. Notice the high peak in the perturbation as ε_c approaches the value -1 .

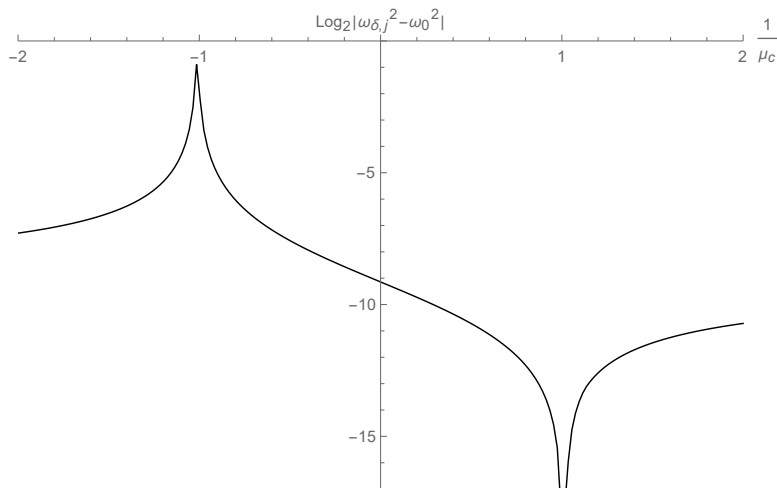


Figure 7: Resonance perturbation $|\omega_{\delta,1}^2 - \omega_0^2|$ as a function of $1/\varepsilon_c$, here allowed to also take negative values.

Finally, suppose we have n particles arranged outside Ω as vertices of a regular n -gon, and tangent to $\partial\Omega$. Suppose all the particles have the same polarization tensor M . As $\delta \rightarrow 0$, we can consider the contribution of each particle independently, and thus summing up (21) we have

$$\omega_{\delta,j}^2 - \omega_0^2 \simeq \sum_{i=1}^n \delta^d \eta_{i,j}, \quad (23)$$

where $\eta_{i,j}$ is the j -th eigenvalue of (22) with z substituted by z_i , the center of the i -th particle. Considering different frequencies, we can reconstruct n by looking for a

minimizer of an appropriate discrepancy functional.

6 Concluding remarks

In this paper, the leading-order term in the shifts of scattering resonances by small particles is derived and the effect of radiation on the perturbations of open cavity modes is characterized. The formula derived characterizes the dependency of the frequency shifts on the position and the polarization tensor of the particle. It is valid for arbitrary-shaped particles. By reconstructing the polarization tensor of the small particle from the shifts of scattering resonances, the orientation of the perturbing particle can be inferred by using the results in [4, Section 4.11.1], which affords the possibility of orientational binding studies in biosensing. It is also worth mentioning that, by combining the arguments of [5, 13] together with those presented here, the formula derived in this paper can be generalized to open electromagnetic and elastic cavities.

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