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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 resonances 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 scattering resonance 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. 35R30, 35C20.

Keywords. Open cavity, Shift of scattering resonances, Whispering-gallery modes, Bio-sensing, Subwavelength resonant particles.

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 [23,39,47]. 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 [52]. 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 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, [21]). Moreover, since it is established only for spherical particles, it cannot 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 [41]. 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. It is worth emphasizing that the Bethe–Schwinger formalism leads to accurate approximations only for eigenvalue problems associated with self-adjoint operators. To develop a more physically accurate approximation, in this paper, the non-Hermitian character of the open cavity problem is fully accounted for since it induces radiation effects or losses; this ultimately yields significantly different approximation formulas from those obtained by employing the Bethe–Schwinger formalism.

In this work, we consider the transverse magnetic polarization case. For the analysis of the transverse electric case we refer the reader to [1]. While the analysis in [1] is mathematically rigorous, the derivations provided here are only formal. A lack of compactness of the operator formulation of the problem is the main obstacle in rigorously proving the approximation formulas obtained in the transverse magnetic case.

Transverse magnetic and electric polarizations can be excited separately in some open cavities, and the shifts in the resonances can be measured efficiently [30,41]. 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 [21]. They can occur in optical cavities possessing a closed concave surface. Spherical, disc, and ring cavities represent the simplest types of resonator geometry, and due to this, they have received much attention in the literature over the years [21]. 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 resonances 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. While a degenerate resonance is associated with multiple scattering modes, an exceptional resonance is a point where both scattering resonances and their corresponding scattering modes coalesce. The order of an exceptional scattering resonance is the size of the associated Jordan block. 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 [24,25,27] for small-amplitude sensitivity analyses of the scattering resonances. Numerical computation of resonances has been addressed, for instance, in [22,29,34,35,44,51].

The paper is organized as follows. In Sect. 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 Sect. 4, we consider the perturbation of whispering-gallery modes by small particles. A formula is obtained for the shifting of the scattering resonances, and it shows that there is a strong enhancement in the scattering resonance shifts in the case of subwavelength resonant particles, which allows for their recognition in spite of their small size. The splitting of scattering resonances of the open cavity of multiplicity greater than one due to small particles is also discussed. In Sect. 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

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 Fig. 1. Here, $a < 0 < b$, $\delta > 0$ is small, and $\mu_m, \mu_c, \varepsilon_m$, and ε_c are positive constants.

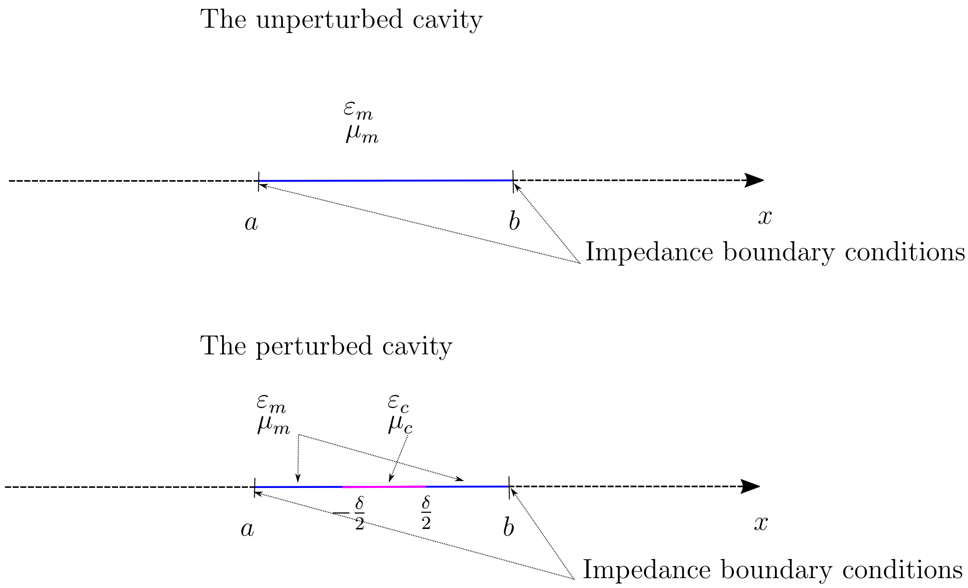

FIG. 1. One-dimensional cavity

Let $\omega_0 \in \mathbb{C}_- := \{z \in \mathbb{C} : \Im z < 0\}$ be a scattering resonance of the unperturbed cavity, and let u_0 denote the corresponding scattering mode, that is,

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

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

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

The above one-dimensional scattering resonance problems govern scattering resonances of slab-type structures [17, Section 1.6]. They are a consequence of Maxwell's equations, under the assumption of time-harmonic solutions. They correspond to the transverse magnetic polarization; see [25]. The scattering resonances ω_0 and ω_δ lie in the lower-half of the complex plane. The scattering modes 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, [22,25].

Proposition 2.1. *As $\delta \to 0$, we have*

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

where

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

The polarization α is defined by

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

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

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

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 2.2. 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, for instance, [6,26], 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:

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

and

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

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

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

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:

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

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

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

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

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

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

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

By the definition of $v^{(1)}$, 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,

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

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,

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

and

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

Therefore,

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

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

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

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

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

where the polarization α is given by

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

Therefore, we arrive at

$$\omega_1 = \frac{\alpha(\partial_x u_0(0))^2}{2\omega_0\mu_m\varepsilon_m \int_a^b u_0^2 \,\mathrm{d}x + i\varepsilon_m((u_0(a))^2 + (u_0(b))^2)}. \tag{6}$$

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. If one employs the Bethe–Schwinger formalism, then one arrives at

$$\omega_1 = \frac{\alpha|\partial_x u_0(0)|^2}{2\omega_0},$$

which differs significantly from (6).

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

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

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

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

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

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

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

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

and so

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

which yields the result. ⋄

Remark 2.3. Proposition 2.1 can be easily generalized to the case where ε_m and μ_m are variable in (a, b). Under the normalization $\int_a^b \varepsilon_m(x)\mu_m(x)|u_0(x)|^2 \, \mathrm{d}x = 1$, the shift in the scattering resonance ω_1 is given by

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

where the polarization α is defined by

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

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

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

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).

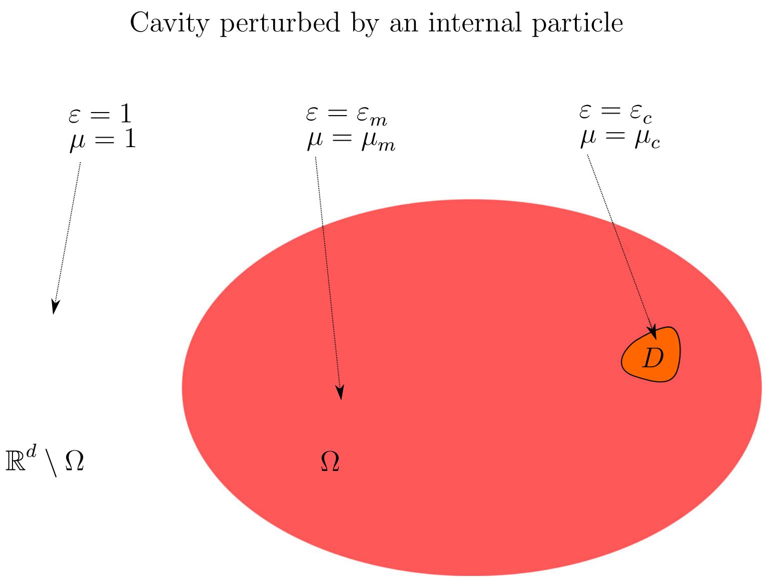

FIG. 2. Multi-dimensional cavity

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 [27]. We use the same notation as in Sect. 2.

Let Ω be a bounded domain in $\mathbb{R}^d$ for $d = 2, 3$, with smooth boundary $\partial\Omega$, see Fig. 2. Let $\omega_0 \in \mathbb{C}_-$ be a simple eigenvalue of the unperturbed open cavity. Then there exists a non-trivial solution u_0 to the equation:

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

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 [22] for a precise statement of the outgoing radiation condition, which for completeness is briefly outlined below.

Remark 3.1. If $d = 2$, then (8) can be obtained from Maxwell's equation in the case where the medium of propagation is invariant along one direction and the propagation of a linearly polarized magnetic field along that direction of invariance is considered [17].

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]

$$T_\omega : \phi = \sum_{m \in \mathbb{Z}} \phi_m e^{im\theta} \mapsto \sum_{m \in \mathbb{Z}} z_m(\omega, R) \phi_m e^{im\theta}, \tag{9}$$

for $d=2$ and by

$$T_\omega : \phi = \sum_{m=0}^{+\infty} \sum_{l=-m}^{m} \phi_m^l Y_m^l \mapsto \sum_{m=0}^{+\infty} z_m(\omega, R) \sum_{l=-m}^{m} \phi_m^l Y_m^l,$$

for $d=3$, 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).

Then the outgoing radiation condition is as follows:

$$(1/\varepsilon_m) \frac{\partial u_0}{\partial \nu} = T_{\omega_0}[u_0] \quad \text{on } \partial\Omega. \tag{10}$$

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

$$\begin{cases} (1/\varepsilon_m)\Delta u_0 + \omega_0^2 \mu u_0 = 0 & \text{in } \Omega, \\ (1/\varepsilon_m) \dfrac{\partial u_0}{\partial \nu} = T_{\omega_0}[u_0] & \text{on } \partial\Omega, \\ \varepsilon_m \mu_m \int\limits_\Omega |u_0|^2 = 1, \end{cases} \tag{11}$$

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 scattering modes grow exponentially at large distances from the cavity since they satisfy the outgoing radiation condition. We also remark that since on the one hand, $z_{-m}(\omega, R) = z_m(\omega, R)$ for all $m \in \mathbb{Z}$, and on the other hand, $Y_m^{-l} = (-1)^l \overline{Y}_m^l$, we have

$$\int\limits_{\partial\Omega} T_\omega[f] g \, d\sigma = \int\limits_{\partial\Omega} f T_\omega[g] \, d\sigma \quad \text{for all } f, g \in H^{1/2}(\partial\Omega), \tag{12}$$

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 is 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 (10), the eigenvalue problem is to find ω_δ such that there is a non-trivial couple $(\omega_\delta, u_\delta)$ satisfying

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

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

Proposition 3.2. *As $\delta \to 0$, we have*

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

where

$$\omega_1 = \frac{M(\varepsilon_m/\varepsilon_c, B)\nabla u_0(z)\cdot\nabla u_0(z) + \omega_0^2|B|\varepsilon_m(\mu_c-\mu_m)(u_0(z))^2}{2\omega_0\mu_m\varepsilon_m\int\limits_\Omega u_0^2\,\mathrm{d}x + \varepsilon_m\int\limits_{\partial\Omega}\partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0\,\mathrm{d}\sigma}, \tag{13}$$

with M being the polarization tensor associated with the domain B and $\varepsilon_m/\varepsilon_c$ the contrast defined by (16) with $v^{(1)}$ being given by (15).

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

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

Let the outer expansion of u_δ be

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

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

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

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

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

Moreover, we obtain

$$\begin{cases} ((1/\varepsilon_m)\Delta + \lambda_0\mu_m)u_1(y) = -\lambda_1\mu_m u_0(y) & \text{for } |y-z| \gg O(\delta), \\ (1/\varepsilon_m)\dfrac{\partial u_1}{\partial\nu} = T_{\omega_0}[u_1] + \omega_1\partial_\omega T_\omega|_{\omega=\omega_0}[u_0] & \text{on } \partial\Omega, \end{cases} \tag{14}$$

and

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

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

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

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 [6])

$$\begin{cases} \Delta_\xi v^{(1)} = 0 & \text{in } \mathbb{R}^d\setminus\bar{B}, \\ \Delta_\xi v^{(1)} = 0 & \text{in } B, \\ \dfrac{\partial v^{(1)}}{\partial\nu}|_+ = (\varepsilon_m/\varepsilon_c)\dfrac{\partial v^{(1)}}{\partial\nu}|_- & \text{on } \partial B, \\ v^{(1)}(\xi) \sim \xi & \text{as } |\xi| \to +\infty. \end{cases} \tag{15}$$

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]

$$M(\varepsilon_m/\varepsilon_c, B) = (\frac{\varepsilon_m}{\varepsilon_c} - 1)\int\limits_{\partial B}\frac{\partial v^{(1)}}{\partial\nu}\big|_-(\xi)\xi\,\mathrm{d}\sigma(\xi). \tag{16}$$

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

$$u_1(y) \sim -M(\varepsilon_m/\varepsilon_c, B)\nabla\Gamma(y-z)\cdot\nabla u_0(z) \quad \text{as } y \to z. \tag{17}$$

Multiplying (14) by u_0 and integrating by parts over $\Omega \setminus \bar{B}_\delta$, we obtain from (12) that

$$-\lambda_1 \mu_m \int\limits_{\Omega\setminus B_\rho} (u_0)^2 \, \mathrm{d}x = \underbrace{\int\limits_{\partial\Omega} \big(T_{\omega_0}[u_1]u_0 - T_{\omega_0}[u_0]u_1\big) \, \mathrm{d}\sigma}_{=0} + \omega_1 \int\limits_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 \, \mathrm{d}\sigma$$
$$+ \frac{1}{\varepsilon_m} \int\limits_{\partial B_\delta} (u_0 \frac{\partial u_1}{\partial \nu} - u_1 \frac{\partial u_0}{\partial \nu}) \, \mathrm{d}\sigma.$$

From (17), we have

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

Therefore,

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

and finally, we arrive at

$$\lambda_1 = \frac{M(\varepsilon_m/\varepsilon_c, B) \nabla u_0(z) \cdot \nabla u_0(z)}{\mu_m \varepsilon_m \int\limits_{\Omega} u_0^2 \, \mathrm{d}x + (1/(2\omega_0))\, \varepsilon_m \int\limits_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 \, \mathrm{d}\sigma}, \tag{18}$$

or equivalently,

$$\omega_1 = \frac{M(\varepsilon_m/\varepsilon_c, B) \nabla u_0(z) \cdot \nabla u_0(z)}{2\omega_0 \mu_m \varepsilon_m \int\limits_{\Omega} u_0^2 \, \mathrm{d}x + \varepsilon_m \int\limits_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 \, \mathrm{d}\sigma}. \tag{19}$$

We then get the desired result. □

In the multi-dimensional case, the effect of radiation on the shift of the scattering resonance ω_0 is given by $\varepsilon_m \int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 \, \mathrm{d}\sigma$. Note also that formula (19) 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 (19) by computing, as in [6] and in Sect. 2, the second-order corrector e_2. As in the one-dimensional case, if one employs the Bethe–Schwinger formalism, then one arrives at

$$\omega_1 = \frac{M(\varepsilon_m/\varepsilon_c, B) \nabla u_0(z) \cdot \nabla \overline{u_0}(z)}{2\omega_0},$$

which is significantly different from (19).

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 [21,33,36,38,39,42,46]. Whispering-gallery modes are exploited to probe the local surroundings [31,32,40]. 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 [14,21,49,50]. 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 $\rho > 0$ and let Ω_ρ be a small neighborhood of Ω, *i.e.*, $\Omega \Subset \Omega_\rho$ and the distance between $\partial\Omega_\rho$ and $\partial\Omega$ is smaller than ρ. Suppose that

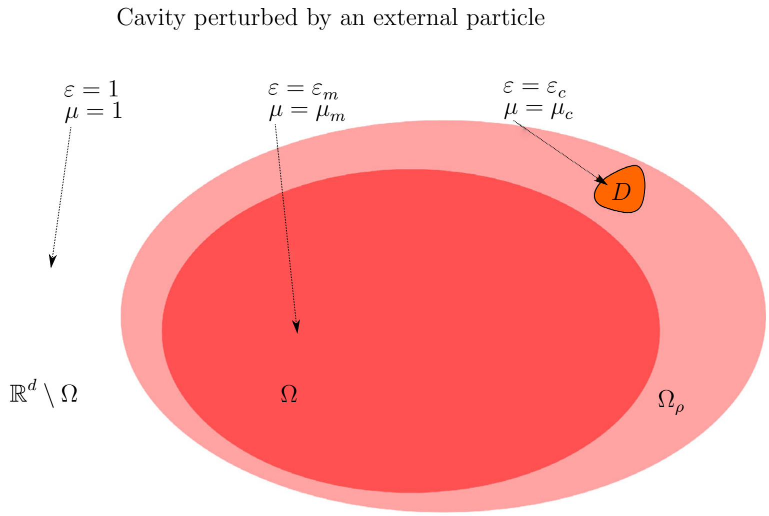

FIG. 3. Perturbed cavity by an external particle

the particle D is in $\Omega_\rho \setminus \overline{\Omega}$, see Fig. 3. If the characteristic size δ of D is much smaller than ρ, which is in turn much smaller than $2\pi/(\sqrt{\varepsilon_m \mu_m}\Re\omega_0)$, then by the same arguments as those in the previous section, we obtain the following result.

Proposition 4.1. *For ρ small enough, the leading-order term in the shift of the scattering resonance ω_0 is given by*

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

Here, the polarization tensor $M(\varepsilon_m/\varepsilon_c, B)$ in (18) 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

$$v_0(x) = -\omega_0^2(\mu_m - 1)\int\limits_\Omega \Gamma(x - y; \omega_0) u_0(y)\,\mathrm{d}y + \left(\frac{1}{\varepsilon_m} - 1\right)\int\limits_\Omega \nabla_y \Gamma(x - y; \omega_0) \cdot \nabla u_0(y)\,\mathrm{d}y, \tag{21}$$

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 resonance yields that the gradient of v_0 at the location of the particle has a significant magnitude.

Remark 4.2. The shift of the scattering resonance is proportional to the volume of the particle and the polarization tensor. Hence, a small particle with a large polarizability can affect significantly the scattering resonances of the cavity.

We can now modify slightly our model to include the case of resonant subwavelength particles (one can think of a metallic nanoparticle for instance). We can assume that D is constituted of a dispersive material such that its dielectric permittivity depends on the operating frequency $\varepsilon_c = \varepsilon_c(\omega)$. If the real part of $\varepsilon_c(\omega)$ takes negative values over a range of frequencies (like for metals at optical frequencies, see [43]), it is well-known that the polarization tensor of the particle becomes frequency dependent and can blow up for a discrete set of frequencies. This phenomenon is known as *plasmonic resonance* of nanoparticles (see [28] for experimental data, and [2,8,11] for a mathematical treatment). At these plasmonic resonance frequencies, problem (15) is nearly singular and therefore the polarization tensor associated with the particle D blows up (see references above).

Assume that the subwavelength resonant particle is coupled to the cavity, *i.e.*, there is a whispering-gallery cavity resonance 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 resonance ω_0 is given by the following proposition.

Proposition 4.3. *We have,*

$$\omega_1 \simeq \frac{M((1/\varepsilon_c)(\Re\omega_0), B)\nabla v_0(z) \cdot \nabla v_0(z) + \omega_0^2 |B|(\mu_c - 1)(v_0(z))^2}{2\omega_0\mu_m\varepsilon_m \int\limits_\Omega u_0^2 \,\mathrm{d}x + \varepsilon_m \int\limits_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 \,\mathrm{d}\sigma}, \tag{22}$$

where v_0 is defined by (21).

Proposition 4.3 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 [12,19,20], ω_0 can be split into m scattering resonances $\omega_{\delta,j}$ having the following approximations:

$$\omega_{\delta,j}^2 \simeq \omega_0^2 + \delta^d \eta_j, \tag{23}$$

with η_j being the j-th eigenvalue of the matrix

$$\left(\frac{M\nabla v_{0,p}(z) \cdot \nabla v_{0,q}(z) + \omega_0^2|B|(\mu_c - 1)v_{0,p}(z)v_{0,q}(z)}{\mu_m\varepsilon_m \int\limits_\Omega u_{0,p}u_{0,q} \,\mathrm{d}x + (1/(2\omega_0))\,\varepsilon_m \int\limits_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_{0,q}]u_{0,p} \,\mathrm{d}\sigma} \right)_{p,q=1}^m. \tag{24}$$

Here, $\{v_{0,q}\}_{q=1,\dots,m}$ are obtained by (21) with $\{u_{0,q}\}_{q=1,\dots,m}$ being an orthonormal eigenspace associated with ω_0.

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 $\delta \to 0$, we can consider the contribution of each particle independently, and thus summing up (23) we have

$$\omega_{\delta,j}^2 - \omega_0^2 \simeq \sum_{i=1}^n \delta^d \eta_{i,j}, \tag{25}$$

where $\eta_{i,j}$ is the j-th eigenvalue of (24) with z substituted by z_i, the center of the i-th particle.

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 [37]. 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 [18]. 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 [45,48].

Throughout this section, we suppose we have a disk-shaped cavity and particle in $\mathbb{R}^2$, with the cavity having radius R and the particle having radius δ. In this case we can obtain almost fully analytic representations of v_0 in (20) and (21) using multipole expansions.

Denote the cylindrical polar counterparts of the Cartesian coordinates (x_1, x_2) and (y_1, y_2) by $(r_x, e^{i\theta_x})$ and $(r_y, e^{i\theta_y})$, respectively. Now $u_0(y)$ is of the form

$$u_0(y) = \sum_{n\in\mathbb{Z}} u_0^n J_n(kr_y)e^{in\theta_y}, \qquad y \in \Omega, \tag{26}$$

and for $x \in \mathbb{R}^2 \setminus \overline{\Omega}$, $y \in \Omega$, we can expand $H_0^{(1)}(\omega_0|x-y|)$ using Graf's addition theorem as

$$H_0(\omega_0|x-y|) = \sum_{n\in\mathbb{Z}} H_n(\omega_0 r_x)e^{in\theta_x} J_n(\omega_0 r_y)e^{-in\theta_y}. \tag{27}$$

Denote by

$$\psi^{(1)}(n,\omega_0,r_x) = \frac{\omega_0}{2}(H_{n-1}^{(1)}(\omega_0 r_x) - H_{n+1}^{(1)}(\omega_0 r_x)),$$
$$\psi^{(2)}(n,\omega_0,r_x) = \frac{in}{r_x}H_n^{(1)}(\omega_0 r_x),$$

and

$$\gamma^{(1)}(n,\omega_0,k,R) := \int_0^R J_n(\omega_0 r_y)J_n(kr_y)r_y \mathrm{d}r_y,$$
$$\gamma^{(2)}(n,\omega_0,k,R)$$
$$:= \int_0^R \left(\frac{\omega_0 k}{4}(J_{n-1}(\omega_0 r_y) - J_{n+1}(\omega_0 r_y))(J_{n-1}(kr_y) - J_{n+1}(kr_y)) + \frac{n^2}{r_y^2}J_n(\omega_0 r_y)J_n(kr_y)\right)r_y \mathrm{d}r_y.$$

Then using (26) and (27) it is easy to show that

$$\begin{aligned} v_0(x) = {} & \frac{i\pi}{2}\sum_{n\in\mathbb{Z}} u_0^n e^{in\theta_x} H_n^{(1)}(\omega_0 r_x) \\ & \times \left(\omega_0^2(\mu_m - 1)\gamma^{(1)}(n,\omega_0,k,R) - (1/\varepsilon_m - 1)\gamma^{(2)}(n,\omega_0,k,R)\right), \end{aligned} \tag{28}$$

$$\begin{aligned} \nabla v_0(x) = {} & \frac{i\pi}{2}\sum_{n\in\mathbb{Z}} u_0^n e^{in\theta_x} \begin{bmatrix}\psi^{(1)}(n,\omega_0,r_x)\\ \psi^{(2)}(n,\omega_0,r_x)\end{bmatrix} \\ & \times \left(\omega_0^2(\mu_m - 1)\gamma^{(1)}(n,\omega_0,k,R) - (1/\varepsilon_m - 1)\gamma^{(2)}(n,\omega_0,k,R)\right). \end{aligned} \tag{29}$$

It is also straightforward, again using (26), to obtain that

$$\int_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_0]u_0 \ \mathrm{d}\sigma = 2\pi \sum_{n\in\mathbb{Z}} u_0^n u_0^{-n}(-1)^n (J_n(kR))^2 g(n,\omega_0,R), \tag{30}$$

where $g(n,\omega_0,R) = g^1(n,\omega_0,R) + g^2(n,\omega_0,R) + g^3(n,\omega_0,R)$ with

$$g^1(n,\omega_0,R) = \frac{-R\omega}{4}\left(\frac{H_{n-1}^{(1)}(\omega_0 R) - H_{n+1}^{(1)}(\omega_0 R)}{H_n(\omega_0 R)}\right)^2,$$

$$g^2(n,\omega_0,R) = \frac{1}{2}\frac{H_{n-1}^{(1)}(\omega_0 R) - H_{n+1}^{(1)}(\omega_0 R)}{H_n^{(1)}(\omega_0 R)},$$

$$g^3(n,\omega_0,R) = \frac{R\omega_0}{4}\left(\frac{H_{n-2}^{(1)}(\omega_0 R) + 2H_n^{(1)}(\omega_0 R) + H_{n+2}^{(1)}(\omega_0 R)}{H_n^{(1)}(\omega_0 R)}\right).$$

We compute 'true' resonances ω_δ using the multipole expansion method in conjunction with a projective eigensolver and Muller's method. To verify the asymptotic formula for ω_1 (20) we use the following parameters that describe both a permittivity and permeability contrast: $\varepsilon_m = 2.3,\ \mu_m = 0.2$ (cavity), $\varepsilon = 1,\ \mu = 1$ (background), $\varepsilon_c = 5,\ \mu_c = 0.5$ (particle). We position the cavity at the origin and set its radius to $R = 1.3$.

Locating a particle next to the cavity splits ω_0 into two scattering resonances $\omega_{\delta,q}$ where $q \in \{1, 2\}$ which have associated orthonormal eigenspaces; see (24) and Fig. 4 which shows how these perturbed resonances approach the unperturbed resonance as $\delta \to 0$ when the particle is positioned at $z = (1.32, 0)$. In this figure, and the following figures, ω_1 is given by asymptotic formula (20) with v_0 and ∇v_0 computed using (28) and (29) and the integral in the denominator computed using (30).

We now refer to $\omega_{\delta,1}$ and $\omega_{\delta,2}$ as simply the perturbed resonance ω_δ where it should be understood that a choice of associated orthonormal eigenspace has been made. In Fig. 5 we position the particle at $z = (z_1, 0)$ with $z_1 \in [1.5, 4]$ and compare the true perturbation $\omega_\delta - \omega_0$ computed numerically, with the predicted perturbation $\delta^2\omega_1$, for whispering gallery modes '6' and '10' (WGM-6 and WGM-10). It can be seen that the asymptotic formula matches up with the numerically computed resonance shift very closely allowing us to easily reconstruct δ from a single scattering resonance shift.

The fact that the perturbation $\delta^2|\omega_1|$ is increasing in Fig. 5 for WGM-6, yet decreasing for WGM-10 is due to the fact we have chosen the $q = 1$ eigenspace for WGM-6 and $q = 2$ eigenspace for WGM-10 in these plots. The field plots in Fig. 5 show solutions to (11), *i.e.*, the unperturbed problem formulated in terms of the capacity operator defined by (9).

It is also possible to reconstruct the polarization tensor using the asymptotic perturbation formulas. Note that a strong enhancement in the scattering resonance shift allows for the recognition of much smaller particles. In Fig. 6 we again compare the true perturbation with the perturbation predicted by asymptotic formula (20) for WGM-6, this time positioning the particle at $z = (1.5, 0)$ and considering $1/\varepsilon_c \in [-2, 2]$. Note the high peak at $1/\varepsilon_c = 1$, indicating a powerful scattering resonance shift, due to the blow-up of the polarization tensor.

We now consider the multiple particle case, specifically validation of resonance perturbations formulas (23) and (24) and a simple example of how they characterize system information. We again set the cavity radius to $R = 1.3$ and the radius of the particles to $\delta = 0.01$. Suppose we want to recover the number of particles $\hat{n}$ that are located at a distance $d = 1.32$ from the origin, *i.e.*, just outside the cavity, if we know that they are arranged into the shape of an $\hat{n}$-gon tangent to the cavity boundary. We also assume we know the material parameters and that these parameters are the same as stated above for the single particle case. We choose $\hat{n} = 5$ in this example, and hence the surrounding particles form a pentagon as can be seen in Fig. 7.

Once again, the nearby particles split the cavity resonance into two modes and it suffices to consider the multiple particle perturbation formulas for one of these modes. In the case of a disk-shaped cavity the matrix in (23) becomes diagonal due to symmetry properties of the multipole coefficients $u^n_{0,1}$ and $u^n_{0,2}$ of the orthogonal eigenspaces $u_{0,1}$ and $u_{0,2}$ which are used to construct $v_{0,1}$ and $v_{0,2}$. In light of this simplification we solve the following minimization problem, featuring a discrepancy functional $J(n)$ given by

$$J(n) = J(n; \omega_\delta, \omega_0, \delta, p) := \left|\omega_\delta - \omega_0 - \delta^2 \sum_{i=1}^{n} \omega_{1,i,p}\right|, \tag{31}$$

where

$$\omega_{1,i,p} = \frac{M(1/\varepsilon_c, B)\nabla v_{0,p}(z_i) \cdot \nabla v_{0,p}(z_i) + \omega_0^2|B|(\mu_c - 1)(v_{0,p}(z_i))^2}{2\omega_0\mu_m\varepsilon_m \int\limits_{\Omega} u_{0,p}^2\,\mathrm{d}x + \varepsilon_m \int\limits_{\partial\Omega} \partial_\omega T_\omega|_{\omega=\omega_0}[u_{0,p}]u_{0,p}\,\mathrm{d}\sigma},$$

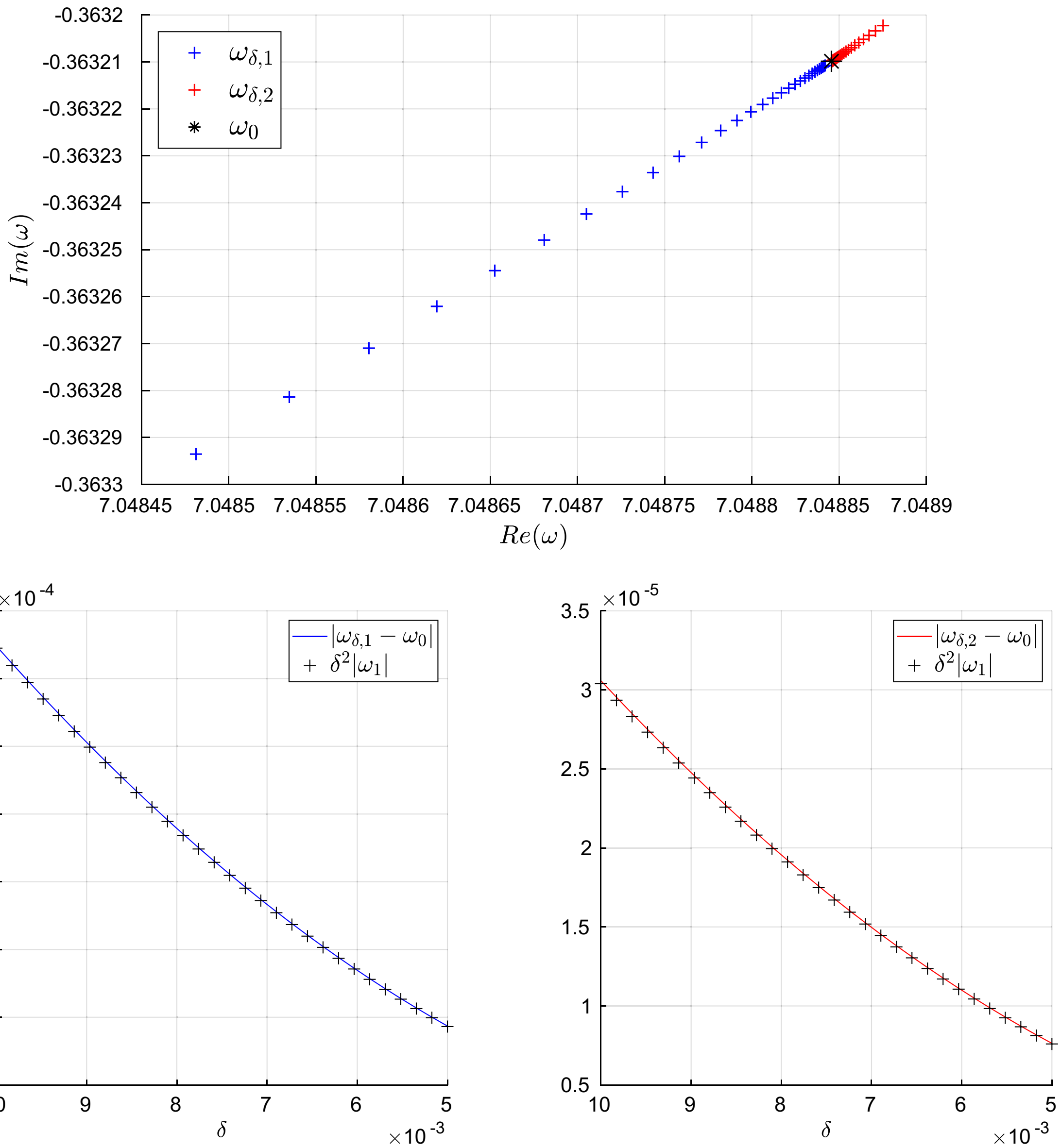

Fig. 4. (Top) As the size of the particle $\delta \to 0$, the perturbed whispering-gallery modes $\omega_{\delta,1}$ and $\omega_{\delta,2}$ converge toward the unperturbed mode ω_0. (Bottom) Absolute values of the true resonance perturbations $\omega_{\delta,1} - \omega_0$ and $\omega_{\delta,2} - \omega_0$ computed numerically (lines) compared with the predicted perturbations (crosses) given by asymptotic formula (20) as the particle size δ decreases. Note a different orthonormal eigenspace has been chosen for ω_1 in the left and right plots

with $p \in \{1, 2\}$, to find the number of particles $\hat{n}$ surrounding the cavity:

$$\hat{n} = \underset{n \in \mathbb{N}_+}{\operatorname{argmin}} \ J(n). \tag{32}$$

We compute $v_{0,p}$ and $\nabla v_{0,p}$ using (28) and (29), respectively, and the integral in the denominator using (30). A simple brute force approach is sufficient to find the $\hat{n}$ satisfying (32) as in the example considered

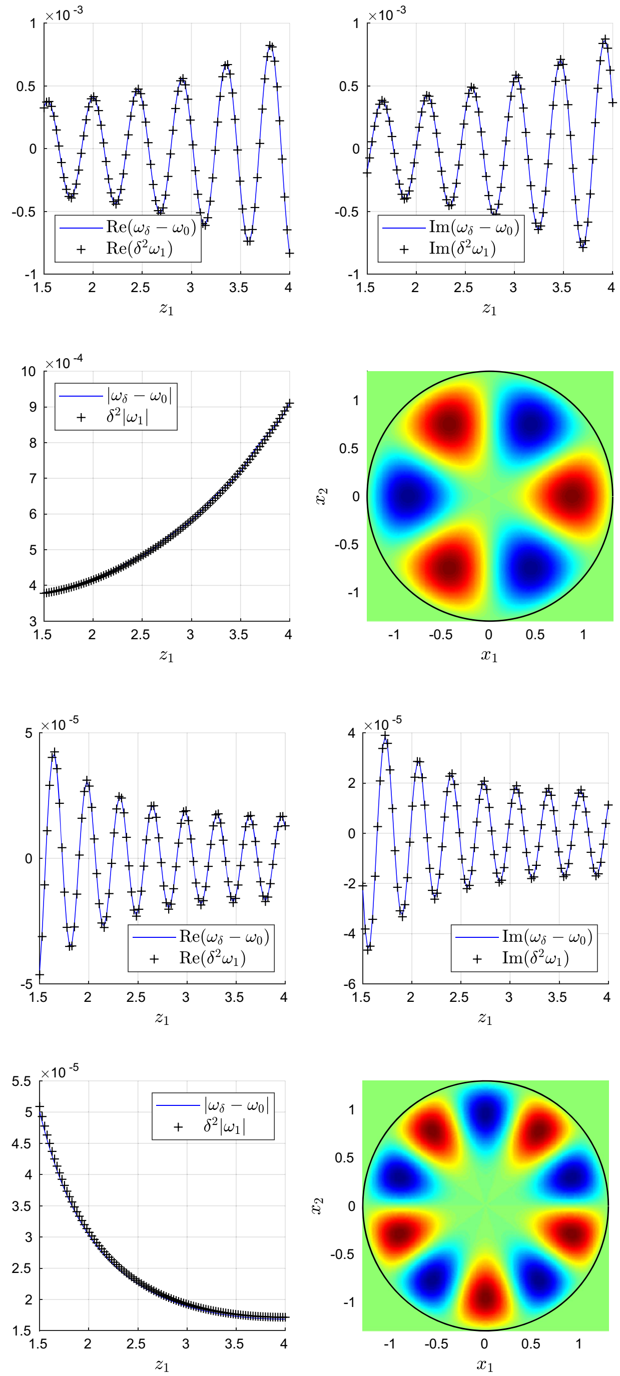

Fig. 5. Real, imaginary, and absolute values of the true resonance perturbation $\omega_\delta - \omega_0$ (blue lines) computed numerically and the predicted perturbation $\delta^2\omega_1$ (black crosses) with ω_1 given by asymptotic formula (20) for whispering-gallery modes '6' and '10'. Here we vary the position $z = (z_1, 0)$ of the particle, *i.e.*, $z_1 \in [1.5, 4]$ (Color figure online)

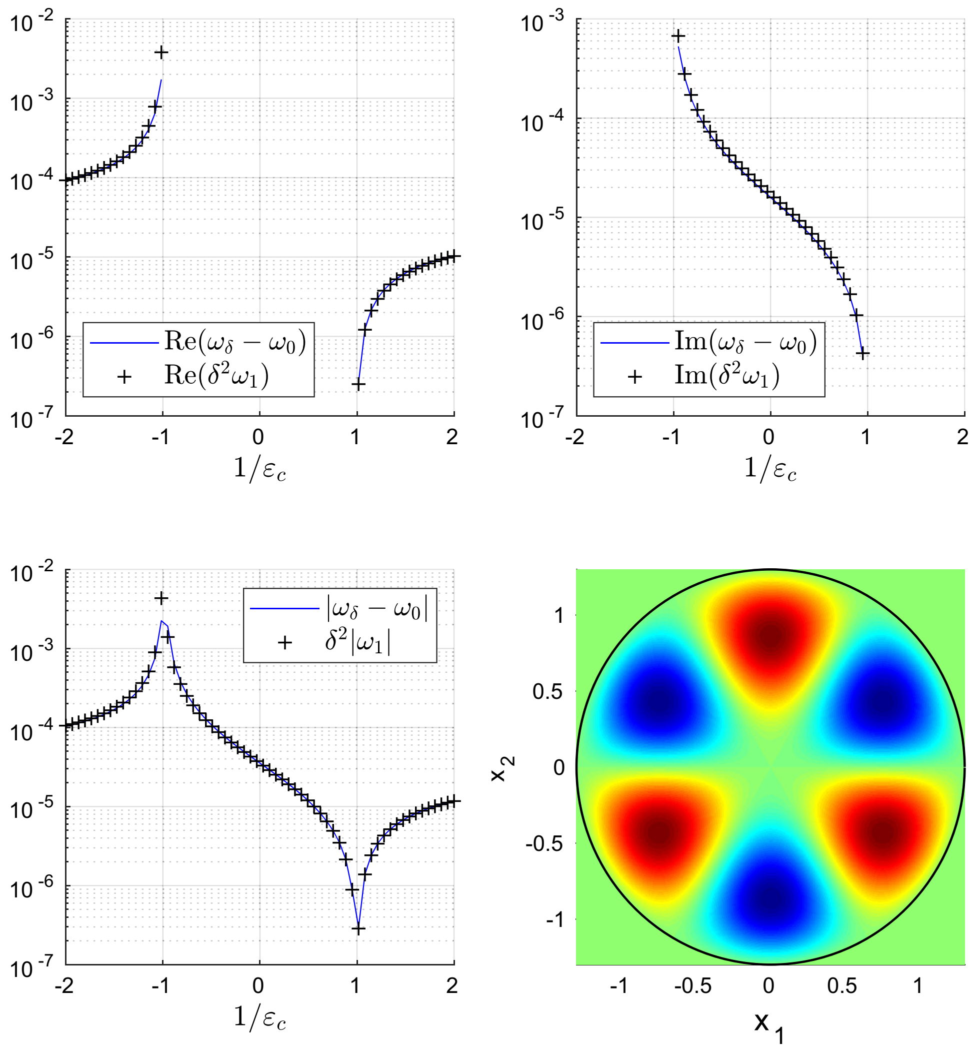

FIG. 6. Comparison between the true resonance perturbation $\omega_\delta - \omega_0$ (blue lines) and the predicted perturbation $\delta^2\omega_1$ (black crosses) with ω_1 given by asymptotic formula (20). Here we vary the inverse of the particle permittivity ε_c, *i.e.*, $1/\varepsilon_c \in [-2, 2]$ (Color figure online)

we are attempting to recover a pentagon. In Table 1 we provide evaluations of $J(n)$ for $n = 1, \ldots, 10$, where it can be seen that $J(n)$ is at least an order of magnitude lower at $n = 5$ than at $n \neq 5$, allowing us to conclude that the cavity is indeed surrounded by $\hat{n} = 5$ particles arranged as a pentagon.

As we have used $\hat{n} = 5$ particles arranged in the shape of a pentagon, $J(n)$ is minimized at $n = 5$

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 scattering resonance shifts on the position and the polarization tensor

Table 1. *Evaluations of the discrepancy functional $J(n)$ in (32) obtained from multiple particle scattering resonance perturbation formulas (23) and (24) for a range of values of n*

n	$J(n)$	n	$J(n)$
1	1.0×10^{-3}	6	2.2×10^{-4}
2	1.1×10^{-3}	7	4.2×10^{-4}
3	3.9×10^{-4}	8	1.4×10^{-3}
4	1.2×10^{-3}	9	8.2×10^{-4}
5	3.0×10^{-5}	10	1.0×10^{-3}

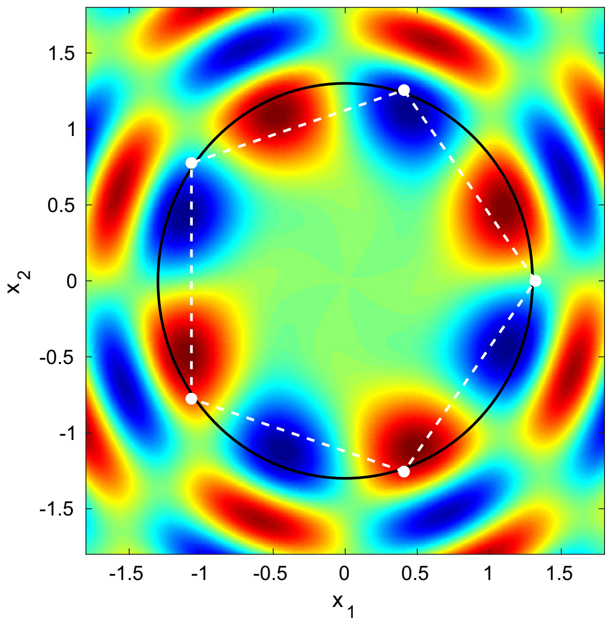

Fig. 7. A cavity (black circle) of radius $R = 1.3$ surrounded by particles (white dots) of radius $\delta = 0.01$ located a distance $d = 1.32$ from the origin and arranged in the shape of a pentagon tangent to the cavity boundary. Minimizing discrepancy functional $J(n)$ (31) allows us to determine the number of particles outside the cavity

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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