Mathematical investigations of resonances in optical micro-resonators

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***Abstract*—We investigate the computation of whispering gallery modes in optical micro-resonators. From a mathematical point of view, this leads to the computation of the complex resonances of dielectric micro-cavities in the sense of the scattering theory. We consider here the 2D case where the scattering problem consists of the Helmholtz equation in $\mathbb{R}^2$ with discontinuities of the normal derivative at the cavity boundary and with the outgoing wave condition at infinity. The computational domain is made finite by the use of *perfectly matched layers* (PML) compatible with the outgoing wave condition, which results in a non self-adjoint problem. Discretization is then achieved by the Finite Element Method. We show theoretical and numerical results for 2D geometries of the micro-cavity.**

***Index Terms*—Scattering resonances, Optical micro-resonators, Finite Element Method, PML**

I. Introduction

An optical micro-resonator is a device basically made of a dielectric cavity (with typical size ranging from one to several hundreds μm) coupled to waveguides or fibers for light input and output [1]. The cavities have a characteristic set of frequencies at which it is possible to confine light-waves when the resonance conditions are met. Light passes through the cavity from the input waveguide and it builds up in intensity over multiple round-trips due to constructive interference. Depending on the optical characteristics of the cavity, it is possible to access a wide range of optical phenomena. Optical micro-resonators came to be important components in the photonic toolbox where they are implemented as lasers, amplifiers, sensors, filters, demultiplexers, switches, routers, logic gates, etc. [2]. However, the theoretical study of optical micro-resonators in order to improve their characteristics, their design or to broaden the field of applications is currently hampered by the weakness of the mathematical models used to describe their functioning and the relative inefficiency of the numerical simulation tools available.

In this work we investigate from a mathematical point of view the scattering problem associated with the computation of optical resonances in a micro-cavity for a 2D setting. The resonances are numerically computed by solving the scattering problem (detailed in Section II) by the Finite Element Method (FEM). The outgoing wave condition is handled by the use of a proper Perfectly Matched Layer (PML) presented in Section III. The properties of the PML for our scattering problem are investigated in Section IV in the particular case of a ring-shaped cavity where analytical expressions for the resonances are known. We conclude with numerical simulation results in Section V.

II. The scattering problem

We consider the resonance cavity alone with invariance in the z direction. So we can assume that the optical index and the electro-magnetic field $(\mathbf{E}, \mathbf{H})$ depend only on (x, y). We denote by Ω the open connected set in $\mathbb{R}^2$ filled by the dielectric cavity. We denote by ε_c the dielectric permittivity of the cavity and by n_c its optical index such that $\varepsilon_c = \varepsilon_0 \, n_c^2$ where ε_0 is the dielectric permittivity of vacuum. We also denote by Σ the boundary of Ω and by Ω' the exterior domain ($\Omega' = \mathbb{R}^2 \setminus \overline{\Omega}$) assumed to be vacuum. The optical index is the piecewise constant function n such that $n = n_c$ in Ω and $n = 1$ in Ω'.

Under the z invariance assumption, it is well known that the set of harmonic Maxwell's equations can be split into two sub-systems of equations referred to as transverse electric (TE) equations corresponding to $\mathbf{H} = (0, 0, H_z)$ and transverse magnetic (TM) equations corresponding to $\mathbf{E} = (0, 0, E_z)$. The two subsystems being very similar, we will only consider here the (TE) case. Taking as main unknown the component $u = H_z$ of the magnetic field, the formulation of the resonance

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problem for TE modes reads: find $(k_0, u) \in \mathbb{C} \times \mathrm{H}^2_{\mathrm{loc}}(\mathbb{R}^2 \setminus \Sigma)$ with $u \neq 0$ such that

$$\operatorname{div}\left(n^{-2}\nabla u\right) + k_0^2\, u = 0 \quad \text{in } \Omega \text{ and } \Omega' \tag{1a}$$

$$[u] = 0 \text{ and } \left[n^{-2}\,\partial_\nu u\right] = 0 \quad \text{across } \Sigma \tag{1b}$$

with a radiation condition at infinity that imposes that u has, outside any disk $D(0, R)$ which contains Ω, an expansion in terms of Hankel functions of the first kind $\mathrm{H}^{(1)}_m$ of the following form in polar coordinates (r, θ):

$$u(r, \theta) = \sum_{m\in\mathbb{Z}} c_m\, \mathrm{H}^{(1)}_m(k_0 r)\, \mathrm{e}^{\mathrm{i}m\theta} \quad \forall\theta \in \mathbb{R}/2\pi\mathbb{Z}. \tag{1c}$$

This radiation condition describes outgoing time-harmonic waves for the time dependence $\mathrm{e}^{-\mathrm{i}k_0 ct}$ where c is the speed of light in vacuum. For real positive k_0, the radiation condition (1c) coincides with the classical Sommerfeld radiation condition for outgoing waves. However it is well known, for example [3], that problem (1) has no solution for $k_0 \in \mathbb{R}^*$ and that the resonances k_0 have a negative imaginary part ($\mathrm{Im}(k_0) < 0$) which describes the damping of the modes u in time.

From a numerical point of view, since problem (1) is set in $\mathbb{R}^2$, an artificial boundary has to be introduced to bound the computational domain. This entails the inherent difficulty of the way of choosing the boundary condition on this artificial boundary to replace the radiation condition (1c) at infinity. We have chosen to use Perfectly Matched Layers (PML) as introduced in [4] for the computation of resonances in open systems.

III. Scattering problem with PML

The PML method consists of a complex scaling [5] and a cut-off at infinity. We use a cylindrical PML with parameters $\sigma_0 > 0$, $r_1 > 0$ as inner radius such that $\Omega \subset D(0, r_1)$, $r_2 > r_1$ as outer radius, and a regularity index $p \in \{0, 1, 2, \dots\}$. To define the complex scaling, we introduce the function $\tilde\sigma \in \mathcal{C}^p(\mathbb{R}_+)$ such that $\tilde\sigma(r) = 0$ for $r \le r_1$, $\tilde\sigma(r) = \sigma_0$ for $r \ge r_2$,

$$\tilde\sigma(r) = \sigma_0\, \frac{\int_{r_1}^{r} (s - r_1)^p\, (r_2 - s)^p\, \mathrm{d}s}{\int_{r_1}^{r_2} (s - r_1)^p\, (r_2 - s)^p\, \mathrm{d}s} \quad \text{for } r_1 < r < r_2, \tag{2}$$

and the following quantities: $\sigma(r) = \tilde\sigma(r) + r\tilde\sigma'(r)$, $\tilde d(r) = 1 + \mathrm{i}\,\tilde\sigma(r)$, $d(r) = 1 + \mathrm{i}\,\sigma(r)$, $d_0 = 1 + \mathrm{i}\sigma_0$.

We set $\widetilde u(r, \theta) = u(\tilde d(r) r, \theta)$. The function $\widetilde u$ satisfies the system (1a,1b) in $D(0, r_1)$. In the PML area for $\mathrm{Im}(d_0 k_0) > 0$, $\widetilde u$ satisfies

$$\widetilde\Delta \widetilde u + k_0^2\, \widetilde u = 0 \quad \text{for } r \in (r_1, +\infty) \setminus \{r_2\} \tag{3a}$$

$$[\widetilde u] = 0 \text{ and } \left[\frac{1}{d}\,\partial_r \widetilde u\right] = 0 \quad \text{for } r \in \{r_1, r_2\} \tag{3b}$$

$$\lim_{r\to+\infty} \widetilde u(r, \theta) = 0 \tag{3c}$$

where, in polar coordinates (r, θ),

$$\widetilde\Delta \widetilde u = \frac{1}{r\tilde d}\frac{\partial}{\partial r}\left(r\frac{\tilde d}{d}\frac{\partial \widetilde u}{\partial r}\right) + \frac{1}{\tilde d^2 r^2}\,\frac{\partial^2 \widetilde u}{\partial \theta^2}.$$

Choosing $r_3 \ge r_2$, we approach $\widetilde u$ by $\widehat u$ that satisfies the system (1a,1b) in $D(0, r_1)$ and

$$\widetilde\Delta \widehat u + \widehat k_0^2\, \widehat u = 0 \quad \text{for } r \in (r_1, r_3) \setminus \{r_2\} \tag{4a}$$

$$[\widehat u] = 0 \text{ and } \left[\frac{1}{d}\,\partial_r \widehat u\right] = 0 \quad \text{for } r \in \{r_1, r_2\} \tag{4b}$$

$$\widehat u = 0 \quad \text{for } r = r_3 \tag{4c}$$

The weak formulation of the eigenvalue problem set in the bounded domain $D(0, r_3)$ reads: find $(\widehat k_0, \widehat u) \in \mathbb{C} \times \mathrm{H}^1_0(D(0, r_3))$ with $\widehat u \neq 0$ and $\mathrm{Im}(\widehat k_0) < 0$ such that $\forall v \in \mathrm{H}^1_0(D(0, r_3))$

$$\int_{D(0,r_3)} n^{-2}\, M\, \nabla\widehat u \cdot \nabla v\, \mathrm{d}x\mathrm{d}y - \widehat k_0^2 \int_{D(0,r_3)} d\, \tilde d\, \widehat u\, v\, \mathrm{d}x\mathrm{d}y = 0 \tag{5}$$

where M is the matrix

$$M = \frac{1}{x^2 + y^2}\begin{pmatrix} x^2\, \frac{\tilde d}{d} + y^2\, \frac{d}{\tilde d} & xy\left(\frac{\tilde d}{d} - \frac{d}{\tilde d}\right) \\ xy\left(\frac{\tilde d}{d} - \frac{d}{\tilde d}\right) & x^2\, \frac{d}{\tilde d} + y^2\, \frac{\tilde d}{d}\end{pmatrix}$$

Problem (5) can then be solved by the Finite Element Method in the usual way. For the present study, we have used the open-source Finite Element Library XLiFE++ [6]

IV. A reference problem

In order to investigate computational issues when solving problem (1) by the FEM using PML, we consider a "reference problem" where the micro-cavity has a ring shape with inner radius r_i and outer radius r_o. For such a geometry, separating the variables in polar coordinates provides analytical expressions for the optical modes. We find that solutions u to problem (1) can be expressed as $u(r, \theta) = \sum_{m\in\mathbb{Z}} u_m(r)\, \mathrm{e}^{\mathrm{i}m\theta}$ where u_m is given in terms of Bessel's functions J_m, Y_m, and $\mathrm{H}^{(1)}_m$ as

$$u_m(r) = \begin{cases} C_1\, \mathrm{J}_m(k_0 r) & \text{if } r < r_i \\ C_2\, \mathrm{J}_m(n_c k_0 r) + C_3\, \mathrm{Y}_m(n_c k_0 r) & \text{if } r \in (r_i, r_o) \\ C_4\, \mathrm{H}^{(1)}_m(k_0 r) & \text{if } r > r_o \end{cases}$$

where the four constants $C_1, \dots, C_4$ are determined by the interface conditions (1b) and the resonance k_0 is obtained by solving the "modal equation"

$$\frac{\dfrac{\mathrm{J}'_m(n_c k_0 r_i)}{n_c\, \mathrm{J}'_m(k_0 r_i)} - \dfrac{\mathrm{J}_m(n_c k_0 r_i)}{\mathrm{J}_m(k_0 r_i)}}{\dfrac{\mathrm{Y}'_m(n_c k_0 r_i)}{n_c\, \mathrm{J}'_m(k_0 r_i)} - \dfrac{\mathrm{Y}_m(n_c k_0 r_i)}{\mathrm{J}_m(k_0 r_i)}} = \frac{\dfrac{\mathrm{J}_m(n_c k_0 r_o)}{\mathrm{H}^{(1)}_m(k_0 r_o)} - \dfrac{\mathrm{J}'_m(n_c k_0 r_o)}{n_c\, \mathrm{H}^{(1)\prime}_m(k_0 r_o)}}{\dfrac{\mathrm{Y}_m(n_c k_0 r_o)}{\mathrm{H}^{(1)}_m(k_0 r_o)} - \dfrac{\mathrm{Y}'_m(n_c k_0 r_o)}{n_c\, \mathrm{H}^{(1)\prime}_m(k_0 r_o)}} \tag{6}$$

If $\sum_{m\in\mathbb{Z}} u_m(r)\, \mathrm{e}^{\mathrm{i}m\theta}$ is a resonance for k_0 then each term $u_m(r)\, \mathrm{e}^{\mathrm{i}m\theta}$ is a resonance for the same k_0. We have conducted numerical experiments on this reference problem to explore the influence of the different parameters involved in the definition of the PML on the accuracy of the computations.

First, we have noted that a much better approximation is obtained by increasing the FE polynomial order rather than increasing the number of elements. We have also observed that the parameter σ_0 in (2) must be chosen carefully: large enough to ensure a good convergence of the approximation, but not too large in which case the convergence rate would be affected. Finally, a better performance is obtained by using the lowest regularity on $\widetilde{\sigma}$ corresponding to $p = 0$ in (2). However, choosing $p = 0$ and $\widetilde{\sigma} \in \mathcal{C}^0([0, r_2])$ requires that the mesh of the domain respects the discontinuity of σ at $r = r_1$. We can choose $r_3 = r_2$, this is simpler to code and does not alter the convergence. Other experiments show that the PML width $r_2 - r_1$ does not need to be large.

V. Numerical simulation results

We present numerical simulations obtained for a ring with inner radius $r_i = 0.3$, outer radius $r_o = 0.5$, and optical index $n_c = 10$. Similar simulations (on disk) can be found in [7], [8]. We compare a 1D calculation (done with FE of order 30 and around 200 dofs—as precise as the analytic formulas presented in the previous paragraph) and a 2D calculation (done with triangular FE of order 6 and around 60000 dofs) of the resonances. Computations were carried out using XLiFE++ [6] with the following PML parameters: $r_1 = 1.1$, $r_2 = r_3 = 1.6$, $\sigma_0 = 5$, $p = 0$. We show on Fig. 1 the optical modes corresponding to the following resonances k_0:

j	m	1D	2D	rel. diff.
1	5	$2.000254 - \mathrm{i}\,10^{-7.859}$	$2.000254 - \mathrm{i}\,10^{-7.726}$	$10^{-6.5}$
1	10	$2.942771 - \mathrm{i}\,10^{-14.09}$	$2.942771 - \mathrm{i}\,10^{-10.64}$	$10^{-7.4}$
1	15	$4.004424 - \mathrm{i}\,10^{-14.79}$	$4.004424 - \mathrm{i}\,10^{-13.79}$	$10^{-7.3}$
2	5	$3.367404 - \mathrm{i}\,10^{-5.329}$	$3.367406 - \mathrm{i}\,10^{-5.336}$	$10^{-6.2}$
2	10	$4.050435 - \mathrm{i}\,10^{-13.44}$	$4.050437 - \mathrm{i}\,10^{-10.23}$	$10^{-6.3}$
2	15	$4.975665 - \mathrm{i}\,10^{-16.82}$	$4.975673 - \mathrm{i}\,10^{-14.14}$	$10^{-5.7}$
3	5	$4.842406 - \mathrm{i}\,10^{-3.657}$	$4.842411 - \mathrm{i}\,10^{-3.670}$	$10^{-5.7}$
3	10	$5.354871 - \mathrm{i}\,10^{-10.89}$	$5.354881 - \mathrm{i}\,10^{-9.789}$	$10^{-5.7}$
3	15	$6.095389 - \mathrm{i}\,10^{-14.27}$	$6.095450 - \mathrm{i}\,10^{-11.60}$	$10^{-5.0}$

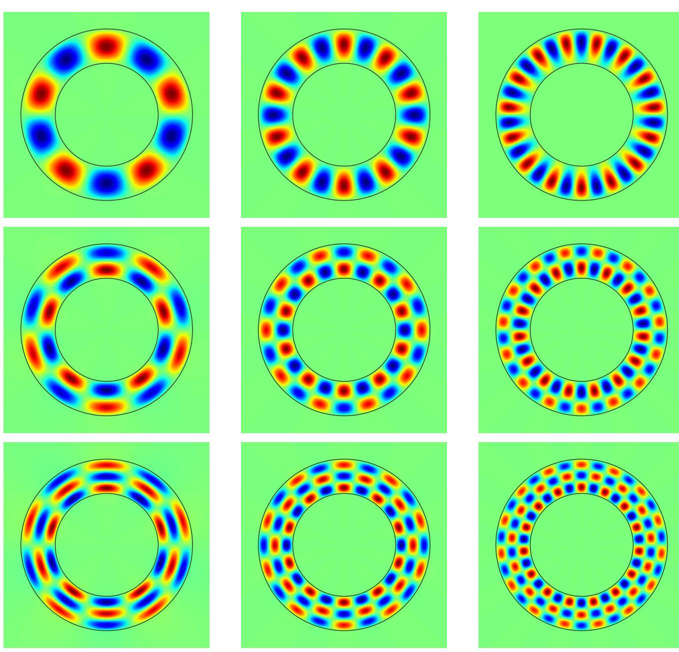

Fig. 1. Optical modes for a ring cavity (real part of the eigenfunction u) for various resonances $k_{0,j}^m$ corresponding to $j = 1, 2, 3$ (row index) and $m = 5, 10, 15$ (column index).

We have also considered a race-track shaped cavity with the following features: length of the straight line 1, external turn radius 0.5, width of the cavity 0.2, and optical index $n_c = 10$. Fig 2 shows the optical mode corresponding to $k_0 = 3.19 - \mathrm{i}\,10^{-4.13}$. Computations were carried out with triangular FE of order 6, around 60000 dofs, and the following PML parameters: $r_1 = 1.1$, $r_2 = r_3 = 1.6$, $\sigma_0 = 5$, $p = 0$.

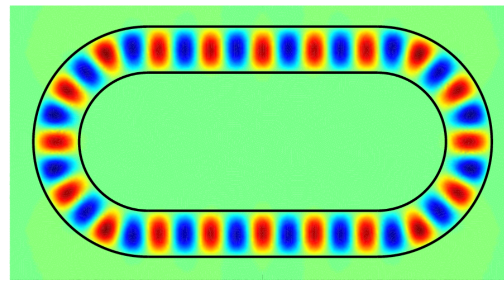

Fig. 2. Optical modes for a race-track shaped cavity (real part of the eigenfunction u) for $k_0 = 3.19 - \mathrm{i}\,10^{-4.13}$.

VI. Conclusion

We have set up a way to compute resonances in 2D dielectric micro-cavity, so we can find resonances on geometries where no analytical solution is available. Furthermore, we know [9] that the resonances have asymptotic expansions as m tends to infinity for a disk. For our computations on the ring, the resonances satisfy the same asymptotic. In a future work, we plan to investigate if there are asymptotic expansions for other geometries.

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