

WGMode toolbox user manual

Stéphane BALAC

Univ. Rennes, CNRS, IRMAR - UMR 6625
F-35000 Rennes, France

`stephane.balac@univ-rennes1.fr`

Release 2.0 - September 2018

Abstract

WGMODE is a MATLAB toolbox aimed at studying Whispering Gallery Modes (WGM) in spherical optical micro-resonators. Whispering gallery modes are specific resonances of an optical wave trapped inside a dielectric cavity with smooth edges due to continuous total internal reflection of light. The novelty of the work stands in the implementation of analytical formulas to compute the volume of a WGM in a spherical cavity while only approximate asymptotic expressions or purely numerical computations based on the Finite Element Method were previously available. The toolbox also provides MATLAB programs to compute and visualize WGM.

Contents

1	Physical and mathematical background	1
2	Numerical issues addressed in the WGMODE toolbox	5
3	WGMODE toolbox contents	7
4	A comprehensive test run under MATLAB	9
5	A comprehensive test run under OCTAVE	17
6	Additional comments	23
	References	25

1 Physical and mathematical background

The WGMODE toolbox provides various MATLAB scripts to study WGM in a spherical optical micro-resonator. For a spherical dielectric cavity, an analytical expression of the electromagnetic field

$$\mathbf{E}(\mathbf{r}, t) = \text{Re}[\underline{\mathbf{E}}(\mathbf{r}) \exp(i\omega t)], \quad \mathbf{B}(\mathbf{r}, t) = \text{Re}[\underline{\mathbf{B}}(\mathbf{r}) \exp(i\omega t)] \quad (1)$$

corresponding to a WGM (ω denotes the resonance frequency) is obtained from Maxwell's harmonic equations using the so-called Hansen's method [1]. We denote by N the optical index of the dielectric cavity and by R its radius. We set $k_0 = \omega/c$ and $k = k_0 N$. Using Hansen's method, it is found that there exists two kinds of electromagnetic field with different polarization

termed TE (transverse electric) and TM (transverse magnetic) defined in spherical coordinates (r, θ, φ) , see Fig. 1, as follows [2, 3]. For TE modes, the mode field can be expressed as

$$\underline{\mathbf{E}}(r, \theta, \varphi) = \begin{cases} \frac{\psi_\ell(kr)}{kr} \mathbf{X}_{\ell m}(\theta, \varphi) & \text{if } r \leq R \\ \frac{k_0}{k} \frac{\psi_\ell(kR)}{\zeta_\ell(k_0R)} \frac{\zeta_\ell(k_0r)}{k_0r} \mathbf{X}_{\ell m}(\theta, \varphi) & \text{if } r > R \end{cases} \quad (2)$$

and

$$\underline{\mathbf{B}}(r, \theta, \varphi) = \begin{cases} \frac{ik}{\omega} \left(\ell(\ell+1) \frac{\psi_\ell(kr)}{k^2 r^2} \mathbf{Z}_{\ell m}(\theta, \varphi) + \frac{\psi'_\ell(kr)}{kr} \mathbf{Y}_{\ell m}(\theta, \varphi) \right) & \text{if } r \leq R \\ \frac{ik_0^2}{k\omega} \frac{\psi_\ell(kR)}{\zeta_\ell(k_0R)} \left(\ell(\ell+1) \frac{\zeta_\ell(k_0r)}{k_0^2 r^2} \mathbf{Z}_{\ell m}(\theta, \varphi) + \frac{\zeta'_\ell(k_0r)}{k_0r} \mathbf{Y}_{\ell m}(\theta, \varphi) \right) & \text{if } r > R \end{cases} \quad (3)$$

where ℓ, m are integers such that $-\ell \leq m \leq \ell$, $\mathbf{X}_{\ell m}$, $\mathbf{Y}_{\ell m}$ and $\mathbf{Z}_{\ell m}$ denote the *Vector Spherical Harmonics* defined from the *Scalar Spherical Harmonics* Y_ℓ^m as

$$\mathbf{Z}_{\ell m} = Y_\ell^m \mathbf{e}_r, \quad \mathbf{Y}_{\ell m} = r \nabla Y_\ell^m, \quad \mathbf{X}_{\ell m} = \nabla Y_\ell^m \wedge \mathbf{r} \quad (4)$$

and ψ_ℓ and ζ_ℓ denote respectively the *Ricatti-Bessel functions* of first and third kinds. They are related to the Bessel function $J_{\ell+\frac{1}{2}}$ and Hankel function $H_{\ell+\frac{1}{2}}^{(2)}$ respectively by [4, 5]

$$\psi_\ell(x) = \sqrt{\frac{\pi x}{2}} J_{\ell+\frac{1}{2}}(x), \quad \zeta_\ell(x) = \sqrt{\frac{\pi x}{2}} H_{\ell+\frac{1}{2}}^{(2)}(x). \quad (5)$$

The Spherical Surface Harmonics of degree ℓ and order m is defined as, see [6],

$$Y_\ell^m(\theta, \varphi) = C_{\ell m} P_\ell^m(\cos(\theta)) e^{im\varphi} \quad -\ell \leq m \leq \ell, \quad \ell \in \mathbb{N} \quad (6)$$

where the normalization constant $C_{\ell m}$ is taken to be

$$C_{\ell m} = \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}. \quad (7)$$

Note that the mode field $(\underline{\mathbf{E}}, \underline{\mathbf{B}})$ given by (2)–(3) is defined up to a normalization constant. Moreover, Hankel function $H_{\ell+\frac{1}{2}}^{(2)}$, and its Riccati-Bessel counterpart ζ_ℓ used in (2)–(3), express outward-propagating spherical-wave solutions of the spherical wave equation for the sign convention $+i\omega t$ used here for the frequency in (1).

For TM modes, we have

$$\underline{\mathbf{E}}(r, \theta, \varphi) = \begin{cases} \ell(\ell+1) \frac{\psi_\ell(kr)}{k^2 r^2} \mathbf{Z}_{\ell m}(\theta, \varphi) + \frac{\psi'_\ell(kr)}{kr} \mathbf{Y}_{\ell m}(\theta, \varphi) & \text{if } r < R \\ \frac{\psi_\ell(kR)}{\zeta_\ell(k_0R)} \left(\ell(\ell+1) \frac{\zeta_\ell(k_0r)}{k_0^2 r^2} \mathbf{Z}_{\ell m}(\theta, \varphi) + \frac{\zeta'_\ell(k_0r)}{k_0r} \mathbf{Y}_{\ell m}(\theta, \varphi) \right) & \text{if } r > R \end{cases} \quad (8)$$

and

$$\underline{\mathbf{B}}(r, \theta, \varphi) = \begin{cases} \frac{ik}{\omega} \frac{\psi_\ell(kr)}{kr} \mathbf{X}_{\ell m}(\theta, \varphi) & \text{if } r \leq R \\ \frac{ik_0}{\omega} \frac{\psi_\ell(kR)}{\zeta_\ell(k_0R)} \frac{\zeta_\ell(k_0r)}{k_0r} \mathbf{X}_{\ell m}(\theta, \varphi) & \text{if } r > R \end{cases} \quad (9)$$

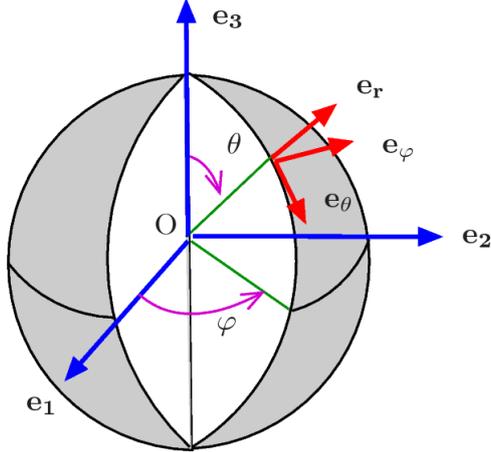


Figure 1: Definition of the spherical coordinate system used.

Here again, the mode field $(\underline{\mathbf{E}}, \underline{\mathbf{B}})$ given by (8)–(9) is defined up to a normalization constant.

Resonance frequencies ω are obtained by solving the so-called *modal equation* [2, 3]

$$P \frac{\psi'_\ell(kR)}{\psi_\ell(kR)} = \frac{\zeta'_\ell(k_0R)}{\zeta_\ell(k_0R)} \quad (10)$$

where $P = N$ for TE modes and $P = 1/N$ for TM modes. As a consequence, a mode is described in terms of three integers: the integer ℓ involved in the modal equation (10), one integer n used to label the solutions of the modal equation (10) for a fixed value of ℓ and the integer m involved in the expression of the electromagnetic field of the mode, see (2)–(3) and (8)–(9). Note that this underscores a mode degeneracy since there exists $2\ell + 1$ modes with the same values of ℓ and n , and therefore with the same resonance frequency ω , but with a different value for m and therefore with a different expression for the electromagnetic field. It can be shown that the *polar mode number* ℓ is equal to the number of wavelengths taken to travel around the sphere and that the *radial mode number* n is equal to the number of intensity maxima of the mode in the radial direction \mathbf{e}_r . The index m is called the *azimuthal mode number*. It can take $2\ell + 1$ values from $-\ell$ to ℓ and it is related to the sinusoidal variation of the mode with the azimuthal angle φ . Negative values of m signifies counter-propagating modes. Moreover, $\ell - |m| + 1$ is the number of intensity maxima in the polar direction \mathbf{e}_θ . Thus modes with index $n = 1$ correspond to the best confined modes in the radial direction and modes for which $m = \ell$ are the best confined in the polar direction. The mode satisfying these conditions and corresponding to the highest value of ℓ for which the modal equation (10) has a solution is termed the *fundamental mode*. WGM refers in the literature to modes with polar index ℓ close to the highest possible value for which the modal equation (10) has a solution, together with a small difference $\ell - |m|$ and n close to unity [2].

Frequencies ω obtained as solutions to the modal equation (10) are complex valued. It is usual in the study of WGM in optical micro-resonators to introduce the *radiative quality factor* as the ratio of the real part of the resonance frequency ω and its imaginary part:

$$Q = \frac{\text{Re}(\omega)}{\text{Im}(\omega)}. \quad (11)$$

The smaller losses by radiation are, the smaller $\text{Im}(\omega)$ is and therefore the higher is the radiative quality factor. We wish to emphasize that the quality factor of an optical micro-resonator usually takes into account other losses phenomena, that can be predominant [7, 8, 2]. Therefore, it is likely to happen that the radiative quality factor is not close to the true, experimentally measured, quality factor.

In practice, spherical optical micro-resonators often correspond to resonators with a large radius compared to the resonance wavelength $\lambda = \omega/c$ of interest in the optical domain. For such resonators, the solutions to the modal equation (10) corresponding to WGM are related to large values of the polar mode index ℓ . For example, if we consider a $50 \mu\text{m}$ radius silica sphere at a wavelength $\lambda \approx 1.5 \mu\text{m}$, we obtain the highest values of ℓ greater than 300, see Section 4. As a consequence, for such a mode the radiative leakage of the energy is small and a good approximation consists in assuming the radiative part outside the sphere as negligible. From a mathematical point of view, this approximation consists in considering the following asymptotic expansions of Bessel's functions for large order ℓ , see e.g. [4, formula 10.19.2] : $\zeta_\ell(z) \approx i\chi_\ell(z)$ where χ_ℓ denotes Riccati-Bessel function of the second kind with order ℓ related to Bessel function $Y_{\ell+\frac{1}{2}}$ by

$$\chi_\ell(x) = -\sqrt{\frac{\pi x}{2}} Y_{\ell+\frac{1}{2}}(x). \quad (12)$$

Analytical formulas for modes volume in spherical optical micro-resonators presented in the next section and implemented in the WGMODE toolbox were obtained under this assumption, mathematically restrictive but very realistic from a practical viewpoint.

This approximation leads to consider the following form for the modal equation

$$P \frac{\psi'_\ell(kR)}{\psi_\ell(kR)} = \frac{\chi'_\ell(k_0R)}{\chi_\ell(k_0R)} \quad (13)$$

that admits real solution k_0 .

The WGMODE toolbox was primarily written to compute the mode volume \mathcal{V} of a WGM in a spherical micro-resonator. The mode volume is defined as the ratio of the total energy stored inside the resonator for that mode and the maximum energy density of the mode [9, Sec. 1.6], [10, Sec. 2.7]:

$$\mathcal{V} = \frac{1}{M} \iiint_{\mathbb{R}^3} \left(\frac{\varepsilon(\mathbf{r})}{2} \|\mathbf{E}(\mathbf{r})\|^2 + \frac{1}{2\mu(\mathbf{r})} \|\mathbf{B}(\mathbf{r})\|^2 \right) d\mathbf{r} \quad (14)$$

where \mathbf{E} and \mathbf{B} are respectively the electric field and magnetic induction of the mode, μ and ε are respectively the magnetic permeability and electric permittivity and $\|\cdot\|$ denotes the euclidean norm in \mathbb{C}^3 . The volume integral is normalized by

$$M = \max_{\mathbf{r} \in \mathbb{R}^3} \left(\frac{\varepsilon(\mathbf{r})}{2} \|\mathbf{E}(\mathbf{r})\|^2 + \frac{1}{2\mu(\mathbf{r})} \|\mathbf{B}(\mathbf{r})\|^2 \right),$$

the maximum of the energy density of the optical mode. Note that the definition (14) of the mode volume is open to question since integrating over the entire space leads to a diverging integral since modes of an optical micro-resonator grow exponentially at infinity. This issue is mostly ignored in the literature and overcome by integrating over a finite integration domain. Such an approach can result in relatively small errors when dealing with modes of high quality factor. We refer to [11] for a detailed discussion of the issue and nevertheless adopt formula (14) as expression of the mode volume. The novelty of the WGMODE toolbox is to provide tools to compute the volume of a WGM in a spherical optical micro-resonator based on an analytical approach to evaluate the volume integral in (14). This ensures both accurate results and fast computation times. Here we make the assumption that the dielectric cavity is non-magnetic, *i.e.* its magnetic permeability μ is the one of vacuum ($\mu = \mu_0$). When we assume that the energy losses by diffraction and diffusion can be neglected, the energy conservation law implies that the contribution of the electric field and the magnetic field to the energy density are equal [12]:

$$\iiint_{\mathbb{R}^3} \frac{\varepsilon(\mathbf{r})}{2} \|\mathbf{E}(\mathbf{r})\|^2 d\mathbf{r} = \iiint_{\mathbb{R}^3} \frac{1}{2\mu_0} \|\mathbf{B}(\mathbf{r})\|^2 d\mathbf{r}. \quad (15)$$

As a consequence, the volume of a WGM is most often computed in the literature from the following formula:

$$\mathcal{V} = \frac{1}{\varepsilon_0 N^2 E_{\max}^2} \iiint_{\mathbb{R}^3} \varepsilon(\mathbf{r}) \|\mathbf{E}(\mathbf{r})\|^2 d\mathbf{r} \quad (16)$$

where E_{\max} denotes the maximum value of the Euclidean norm of the electric field. Formula (16) is well suited for the computation of the mode volume of a TE mode in a spherical optical micro-resonator because of the simple expression of the electric field for TE mode, see (2). It should be noted however that the normalization constant is not the same in (14) and in (16).

For TM modes, computation of the mode volume from (16) is a little more tricky because it is the magnetic induction that has the simplest expression, see (9). Thanks to (15), it is however possible to express the integral in (16) in terms of \mathbf{B} . Unfortunately, the normalization constant in (16) can't be expressed in terms of \mathbf{B} and changing for $\max_{\mathbf{r} \in \mathbb{R}^3} \|\mathbf{B}(\mathbf{r})\|^2$ it would not be consistent when comparing volumes of TE and TM modes. Thus, we will compute the volume of TM mode from the following formula

$$\mathcal{V} = \frac{c^2}{N^2 E_{\max}^2} \iiint_{\mathbb{R}^3} \|\mathbf{B}(\mathbf{r})\|^2 d\mathbf{r} \quad (17)$$

where c is the speed of light in free space.

2 Numerical issues addressed in the WGMODE toolbox

Computation of WGM in a spherical optical micro-resonator must address the following issue. Resonance wavelengths (corresponding to the visible spectrum) are obtained by solving the modal equation (10) that relies on the polar mode index $\ell \in \mathbb{N}$. If one set any value for the integer ℓ , there is a strong possibility that the solutions to the modal equation (10) (if they exist) do not correspond to wavelengths in the visible spectrum and even fewer to WGM. In practice, one is interested by WGM around a given wavelength, say $\lambda \approx 1.5 \mu\text{m}$. However, if one set the value of λ and solves the modal equation (10) for the polar mode index ℓ there will be little chance that the value of ℓ will be an integer. To overcome this issue, we have to proceed in two steps.

1. In a first step, we set the value of the wavelength λ corresponding to a rough approximation of the wavelength of the WGM sought after and we solve the modal equation for the polar mode index ℓ . We obtain a set of solutions that are not integer.
2. In a second step, we choose one of the solution (say the highest for the fundamental mode) and we round it to the nearest integer. We solve once again the modal equation with this integer value of ℓ to determine the resonance wavelengths. Because of the continuity of the solutions to the modal equation with respect to the equation's parameters, the first solution (corresponding to a radial mode index $n = 1$) will be closed to the target value.

Another important issue lies in the solving of the modal equation (10). Indeed, because Riccati-Bessel function of the third kind (just as Hankel's functions) is complex valued, solutions to the modal equation (10) are complex numbers (the imaginary part of which takes into account losses and is required to compute the Q-factor). From a numerical point of view, it is much more difficult to solve a non-linear equation in the complex plane than in the real line. Therefore, we proceed in two steps. We first solve the approximated modal equation (13) on the real line. Then, each real solution of the approximated modal equation (13) is used as an initial guess for the iterative method implemented in the MATLAB `fsolve` routine to solve the modal equation (10). We would like to draw attention to the fact that the solutions to the modal equation (10)

are complex numbers with a very small imaginary part compared to its real part and that solving equation (10) represents a stiff problem from a numerical point of view. The user should pay attention to the information returned by MATLAB `fsolve` routine used to solve equation (10) to decide on the reliability of the radiative quality factor value. Moreover, even if computed accurately, this value can differ significantly from the experimentally measured quality factor because of intrinsic loss sources not taken into account in the radiative quality factor but that can be predominant compared to radiative losses.

For numerical purposes it is more convenient to express the modal equation (13) in terms of Bessel functions of first and second kind. We obtain

$$\frac{Y_{\ell-\frac{1}{2}}(k_0R)}{Y_{\ell+\frac{1}{2}}(k_0R)} - P \frac{J_{\ell-\frac{1}{2}}(kR)}{J_{\ell+\frac{1}{2}}(kR)} = \ell \left(\frac{1}{k_0R} - \frac{P}{kR} \right). \quad (18)$$

For a given mode number ℓ , the wavelengths λ for which resonance occurs are obtained by solving equation (18), that is to say by looking for the zeros of the modal function

$$F_\ell : \lambda \in]0, +\infty[\rightarrow \frac{Y_{\ell-\frac{1}{2}}(k_0R)}{Y_{\ell+\frac{1}{2}}(k_0R)} - P \frac{J_{\ell-\frac{1}{2}}(kR)}{J_{\ell+\frac{1}{2}}(kR)} - \ell \left(\frac{1}{k_0R} - \frac{P}{kR} \right). \quad (19)$$

In the WGMODE toolbox, the zeros of this non-linear function on the real line are computed thanks to MATLAB's `fzero` function. It is very useful from a practical point of view to use the following bounds for the solutions corresponding to WGM provided in [9, p. 25]. For a given λ , the mode numbers ℓ corresponding to solutions to the modal equation (13) are such that

$$\frac{2\pi(R + \delta_P)}{\lambda} < \ell + \frac{1}{2} < N \frac{2\pi(R + \delta_P)}{\lambda} \quad (20)$$

where $\delta_P \approx \frac{\lambda}{2\pi N} \frac{P}{\sqrt{N^2-1}}$. We found by numerical experiments that there is no solution ℓ to (13) greater than the upper bound value in (20) and that there are some solutions lower than the lower bound value, but they do not correspond to WGM. Relation (20) implies that for a fixed value of ℓ the wavelengths λ for which resonance occurs are such that

$$\frac{2\pi R}{\ell + \frac{1}{2} - \alpha} < \lambda < \frac{2\pi RN}{\ell + \frac{1}{2} - \alpha N} \quad (21)$$

where $\alpha = P/(N\sqrt{N^2-1})$. The WGMODE toolbox uses relations (20) and (21) in the root finding process but one can easily ignore these bounds and provide its own bounds by setting the `expert_mode` variable to the value 1 in the main program. In order to be sure to compute all the solutions to the approximated modal equation (13), the interval defined by the above lower and upper bounds is discretized with a very small step-size and sign changes in the values taken by the non-linear function (19) are detected. Then, MATLAB's `fzero` routine is used to accurately compute each solution in the interval it has been located.

To compute the quality factor, one has to solve the exact modal equation (10) in the complex plane. This is achieved by using MATLAB's `fsolve` routine with an initial guess for the iterative algorithm used in `fsolve` given by the (real) solution obtained by solving the approximated modal equation (13) modified by adding a very small imaginary part (MATLAB documentation recommends to set a complex initial point when using the non-linear equation solver `fsolve` in the complex plane). This approach is implemented in the script `qfact.m` of the WGMODE toolbox. Since solving the modal equation (10) amounts to locate the zeros of an analytical function, this can be achieved by computing by quadrature contour integrals in the complex plane according to the Delves-Lyness Method [13, 14]. This approach is implemented in the script `qfactn.m` of the WGMODE toolbox.

A particular attention has been paid to the numerical computation of E_{\max}^2 the maximum value of the euclidean norm of the electric field by optimization methods. Since optimization methods such as the ones implemented in MATLAB `fminunc` routine can't make a distinction between local maxima and the global maximum and because in general convergence is only ensured when the initial guess is sufficiently close to the global maximum, we first have to compute a reliable initial guess. To this purpose, we compare the values of E_{\max}^2 over a coarse grid of the optimization domain (the interval $[0, \pi]$ for TE modes or the set $[0, R] \times [0, \pi]$ for TM modes). Then, the global maximum of E_{\max}^2 is computed by using the `fminunc` routine for unconstrained optimization problem where a Trust Region algorithm is chosen. The Trust Region method requires that the gradient of E_{\max}^2 is provided. Since the `fminunc` routine could sometimes converge to a local maximum, we compare the maximum provided by `fminunc` to the value of the objective function with the initial guess. If the two values differ too much, we consider more reliable and safe to use a brute force method to compute the global maximum that consists in comparing the values of E_{\max}^2 over a very fine grid of the optimization domain. Finally, to overcome the possible absence of the optimization toolbox in the user MATLAB installation, we test if the toolbox is available and if this is not so, we use the above mentioned brute force method to compute the global maximum.

3 WGMODE toolbox contents

The WGMODE toolbox is constituted of various MATLAB scripts aimed at studying WGM in spherical optical micro-resonators. They allow to explore resonance conditions for TE or TM modes, to visualize WGM in a micro-sphere and to compute the volume and quality factor of any given mode. Namely, the WGMODE toolbox contains the following MATLAB scripts :

- ELLRES computes, for a given wavelength, the values of the mode index ℓ for which a resonance occurs (note that the solutions ℓ are real numbers);
- WVLRES computes, for a given polar mode index ℓ the values of the wavelength for which a resonance occurs;
- VOLMOD computes the volume of a whispering gallery mode in a micro-sphere;
- QFACT computes for a given whispering gallery mode its quality factor by solving the modal equation by `fsolve`;
- QFACTN computes for a given whispering gallery mode its quality factor by solving the modal equation by the Delves-Lyness Method;
- PLTMOD plot a whispering gallery mode.

The general organization of the WGMODE toolbox is depicted in Fig. 2. The toolbox also provides a collection of special functions:

- SLEGEND associated Legendre function with Schmidt semi-normalization
- SBESSELJ spherical Bessel function of the first kind
- SBESSELY spherical Bessel function of the second kind
- SBESSELH spherical Bessel function of the third kind (Hankel function)
- DSLEGEND derivative of the associated Legendre function with Schmidt semi-normalization
- DSBESSELJ derivative of the spherical Bessel function of the first kind

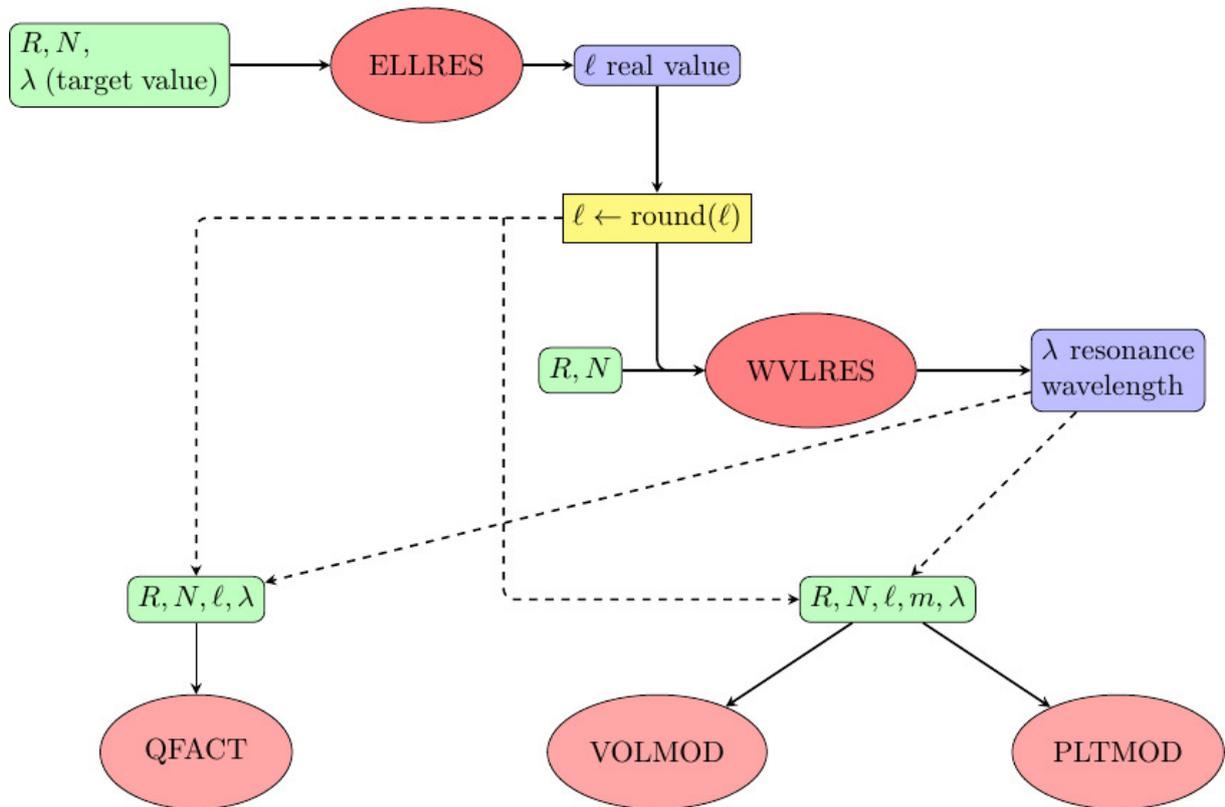


Figure 2: General organization of the WGMODE toolbox. R denotes the sphere radius, N its optical index. λ is the resonance wavelength of the mode and ℓ, m its indexes. The scripts ELLRES and WVLRES are used to compute the resonant mode features around a wavelength target value. The scripts QFACT, VOLMOD can be used to compute key attributes of the mode. PLTMOD allows to display the mode.

- DSBESSELY derivative of the spherical Bessel function of the second kind
- DSBESSELH derivative of the spherical Bessel function of the third kind (Hankel function)
- HANSENM Hansen solution \mathbf{M}_ℓ^m of the spherical vectorial wave equation
- HANSENN Hansen solution \mathbf{N}_ℓ^m of the spherical vectorial wave equation

Lastly, the WGMODE toolbox contains low level internal functions:

- MODEQEL Modal equation (13) for TE or TM modes for a fixed wavelength and a variable mode index
- MODEQWV Modal equation (13) for TE or TM modes for a fixed mode index ℓ and a variable wavelength
- CMODEQWV Modal equation (10) for TE or TM modes for a fixed mode index ℓ and a variable wavelength
- PLOTD plot a discontinuous function removing the draw line at function discontinuity jumps
- VSHNOR computes the square of the euclidean norm of the vector spherical harmonics
- FOPTE/FOPTM objective function (and its gradient) required to compute the maximum of the square of the euclidean norm of the electric field for TE/TM modes
- MODEFIELD computes the electromagnetic field (electric field and magnetic induction) of a given mode
- INTGDL integrand in the Delves-Lyess Method used to solve the modal equation in the complex plane

4 A comprehensive test run under MATLAB

In order to illustrate the use of the WGMODE toolbox, we consider a micro-sphere of radius $50 \mu\text{m}$ and optical index 1.5, see [3]. We are interested in resonance conditions around a wavelength of 1500 nm. First, we use the script entitled `ellres` to determine the solutions ℓ to the approximated modal equation (13) for wave numbers k and k_0 corresponding to a wavelength of 1500 nm and to a TE mode.

```
>> ellres
Micro-sphere radius [micro-m] = 50
Optical index of the micro-sphere = 1.5
Wavelength [nm] = 1500
TE or TM mode ? (TE/TM) : TE

Polar mode indexes ell:

| 1 | 302.418 |           | 7 | 261.233 |           | 13 | 233.160 |
| 2 | 293.024 |           | 8 | 256.086 |           | 14 | 228.991 |
| 3 | 285.350 |           | 9 | 251.163 |           | 15 | 224.932 |
| 4 | 278.578 |           | 10 | 246.432 |           | 16 | 220.977 |
| 5 | 272.399 |           | 11 | 241.867 |           | 17 | 217.125 |
| 6 | 266.649 |           | 12 | 237.448 |           | 18 | 213.356 |
```

Note that an expert mode can be activated by setting the variable `expert_mode` to 1 in the `ellres` program. It provides a plot of the modal function

$$F_\lambda : \ell \in]0, +\infty[\mapsto \frac{Y_{\ell-\frac{1}{2}}(k_0 R)}{Y_{\ell+\frac{1}{2}}(k_0 R)} - P \frac{J_{\ell-\frac{1}{2}}(kR)}{J_{\ell+\frac{1}{2}}(kR)} - \ell \left(\frac{1}{k_0 R} - \frac{P}{kR} \right) \quad (22)$$

the zero of which are the sought out solutions.

The use of the `ellres` program in expert mode is illustrated below.

```
>> ellres
Micro-sphere radius [micro-m] = 50
Optical index of the micro-sphere = 1.5
Wavelength [nm] = 1500
TE or TM mode ? (TE/TM) : TE
Interval of interest for the mode indices search : [0,400]

Polar mode indexes ell:

| 1 | 302.418 |   | 12 | 237.448 |   | 23 | 192.474 |   | 34 | 117.601 |
| 2 | 293.024 |   | 13 | 233.160 |   | 24 | 188.008 |   | 35 | 102.998 |
| 3 | 285.350 |   | 14 | 228.991 |   | 25 | 179.856 |   | 36 | 101.919 |
| 4 | 278.578 |   | 15 | 224.932 |   | 26 | 179.120 |   | 37 | 83.043 |
| 5 | 272.399 |   | 16 | 220.977 |   | 27 | 172.073 |   | 38 | 82.172 |
| 6 | 266.649 |   | 17 | 217.125 |   | 28 | 162.992 |   | 39 | 58.269 |
| 7 | 261.233 |   | 18 | 213.356 |   | 29 | 153.806 |   | 40 | 57.643 |
| 8 | 256.086 |   | 19 | 209.592 |   | 30 | 144.593 |   | 41 | 56.297 |
| 9 | 251.163 |   | 20 | 205.607 |   | 31 | 131.986 |   | 42 | 54.794 |
| 10 | 246.432 |   | 21 | 198.865 |   | 32 | 131.141 |   | 43 | 54.364 |
| 11 | 241.867 |   | 22 | 193.670 |   | 33 | 118.400 |
```

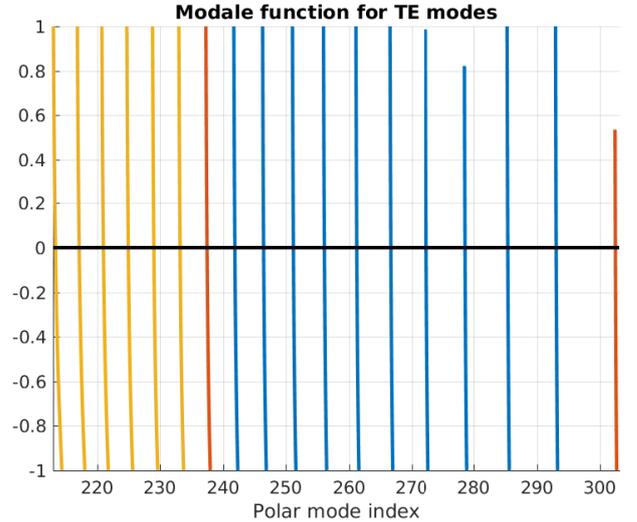
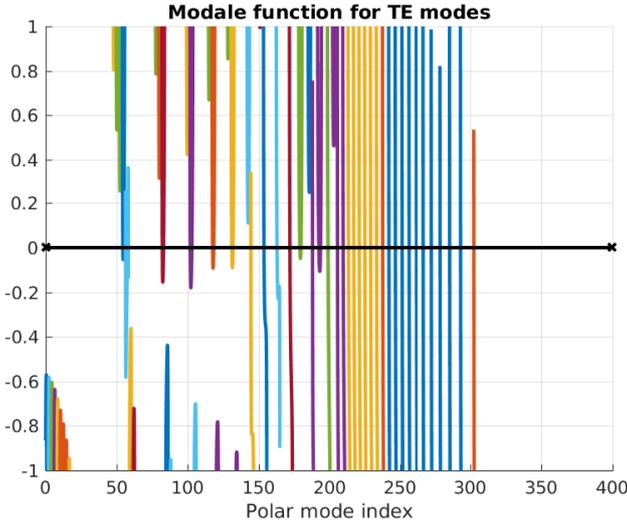


Figure 3: Modal function F_λ defined in (22) for $\lambda = 1500\text{nm}$ over the interval $[0, 400]$ on the left and zoom on the interval $[213, 303]$ on the right.

As can be seen above, the mode indexes ℓ obtained as solutions to the modal equation (10) are not integers. Thus, we have to round up the values to the nearest integer. But doing so, the couple (λ, ℓ) doesn't anymore satisfies the modal equation. For each rounded values for ℓ ,

we have to compute the resonance wavelength by solving once again the modal equation. This time, ℓ is fixed and we look for λ . Computation is achieved with the MATLAB script named `wvlres`. As an example, we consider the first value for ℓ (302.418), rounded to 302.

```
>> wvlres
Micro-sphere radius [micro-m] = 50
Optical index of the micro-sphere = 1.5
Mode index ell = 302
TE or TM mode ? (TE/TM) : TE

Wavelength intervalle of interest found [nm] = [1041.6229 , 1564.7545]

Radial mode number and resonance wavelength [nm]:

| 1 | 1502.024424 |      | 10 | 1260.273611 |      | 19 | 1128.758252 |
| 2 | 1457.369250 |      | 11 | 1242.923923 |      | 20 | 1116.755046 |
| 3 | 1422.192876 |      | 12 | 1226.431024 |      | 21 | 1105.138953 |
| 4 | 1392.096286 |      | 13 | 1210.700903 |      | 22 | 1093.888044 |
| 5 | 1365.368812 |      | 14 | 1195.656160 |      | 23 | 1082.984747 |
| 6 | 1341.115707 |      | 15 | 1181.232108 |      | 24 | 1072.412699 |
| 7 | 1318.793286 |      | 16 | 1167.373999 |      | 25 | 1062.143903 |
| 8 | 1298.039229 |      | 17 | 1154.035012 |      | 26 | 1052.121851 |
| 9 | 1278.596368 |      | 18 | 1141.174768 |      | 27 | 1042.266580 |
```

An expert mode can be activated by setting the variable `expert_mode` to 1 in the `wvlres` program. It allows to compare the resonance wavelengths to the one obtained from the Eikonale approach, see e.g. [3, 9], which basically relies on asymptotic expansion for Bessel's functions of large order. It also provides a plot of the modal function F_ℓ defined by

$$F_\ell : \lambda \in]0, +\infty[\mapsto \frac{Y_{\ell-\frac{1}{2}}(k_0 R)}{Y_{\ell+\frac{1}{2}}(k_0 R)} - P \frac{J_{\ell-\frac{1}{2}}(kR)}{J_{\ell+\frac{1}{2}}(kR)} - \ell \left(\frac{1}{k_0 R} - \frac{P}{kR} \right) \quad (23)$$

the zero of which are the sought out solutions.

```
>> wvlres
Micro-sphere radius [micro-m] = 50
Optical index of the micro-sphere = 1.5
Mode index ell = 302
TE or TM mode ? (TE/TM) : TE
Interval of interest for the wavelength search [nm]: [1040,1600]

Radial mode number and resonance wavelength [nm]:

| 1 | 1502.024424 |      | 10 | 1260.273611 |      | 19 | 1128.758252 |
| 2 | 1457.369250 |      | 11 | 1242.923923 |      | 20 | 1116.755046 |
| 3 | 1422.192876 |      | 12 | 1226.431024 |      | 21 | 1105.138953 |
| 4 | 1392.096286 |      | 13 | 1210.700903 |      | 22 | 1093.888044 |
| 5 | 1365.368812 |      | 14 | 1195.656160 |      | 23 | 1082.984747 |
| 6 | 1341.115707 |      | 15 | 1181.232108 |      | 24 | 1072.412699 |
| 7 | 1318.793286 |      | 16 | 1167.373999 |      | 25 | 1062.143903 |
| 8 | 1298.039229 |      | 17 | 1154.035012 |      | 26 | 1052.121851 |
| 9 | 1278.596368 |      | 18 | 1141.174768 |      | 27 | 1042.266580 |

Compare results to the Eikonale equation ? [y/n] : y
```

Radial mode number and resonance wavelength from the Eikonale equation [nm]:

1	1503.055224	10	1275.318420	19	1158.248551
2	1459.367360	11	1259.647429	20	1147.739023
3	1425.603936	12	1244.819012	21	1137.589781
4	1397.066421	13	1230.736727	22	1127.776064
5	1371.970312	14	1217.321303	23	1118.275745
6	1349.387338	15	1204.506580	24	1109.068956
7	1328.754707	16	1192.236621	25	1100.137776
8	1309.697904	17	1180.463600	26	1091.465969
9	1291.951468	18	1169.146228	27	1083.038776

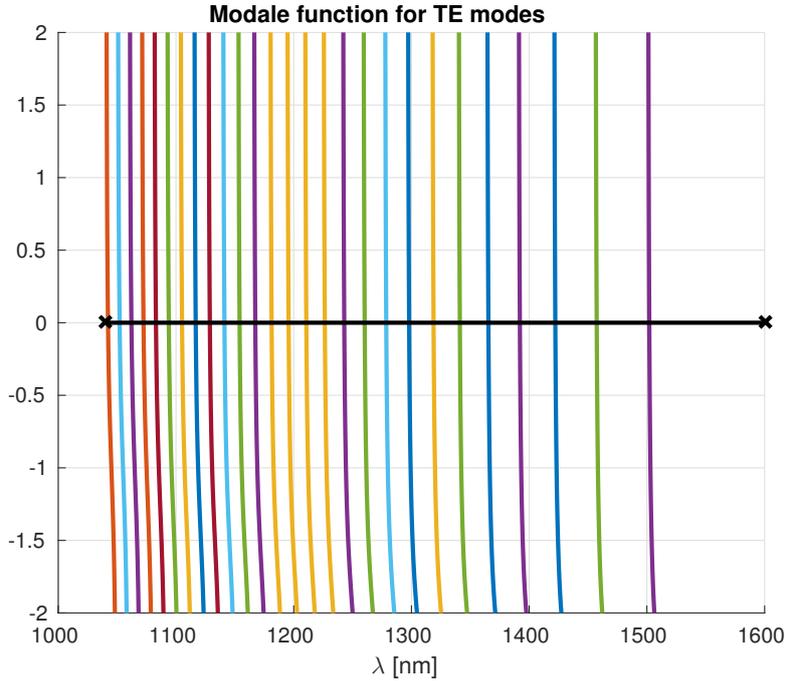


Figure 4: Modal function F_ℓ defined in (23) for $\ell = 302$ and $\lambda \in [1040, 1600]$.

It is possible thanks to the `pltmod` script in the `WGMODE` toolbox to draw the WGM field. Three different plots of the euclidean norm of the electric field $\|\underline{\mathbf{E}}(r, \theta, \varphi)\|$ and magnetic induction $\|\underline{\mathbf{B}}(r, \theta, \varphi)\|$ are proposed. They correspond to a 1D-plot in the radial direction, to a 2D-plot in an azimuthal plane $\varphi = \text{cste}$ and to a 2D-plot in a polar plane $\theta = \text{cste}$. We have depicted in Fig. 5 the radial variation of the electric field and magnetic induction for $(\theta, \varphi) = (\frac{\pi}{2}, 0)$ corresponding to the TE mode with polar index $\ell = 302$ and radial index $n = 5$. It has a resonance wavelength of 1365.36812 nm. Note that the unit is arbitrary since the mode field is defined up to a multiplicative constant. One can clearly see in the figure the five expected maxima in the radial direction for a mode with radial index $n = 5$. One can observe that both the electric field and magnetic induction are continuous across the sphere border as expected for TE modes. This would not be the case for a TM mode.

```
>> pltmod
Micro-sphere radius [micro-m] R = 50
```

```

Optical index of the micro-sphere = 1.5
TE or TM mode : TE
Wavelength [nm] = 1365.36812
Mode number ell = 302
Mode number m = 302
Drawing options :
(A) 1D-plot in the radial direction
(B) 2D-plot in an azimuthal plane phi=cste
(C) 2D-plot in a polar plane theta=cste
Your choice (A/B/C) = A
Minimum radial distance (% value of R) = 80
Maximal radial distance (% value of R) = 110

```

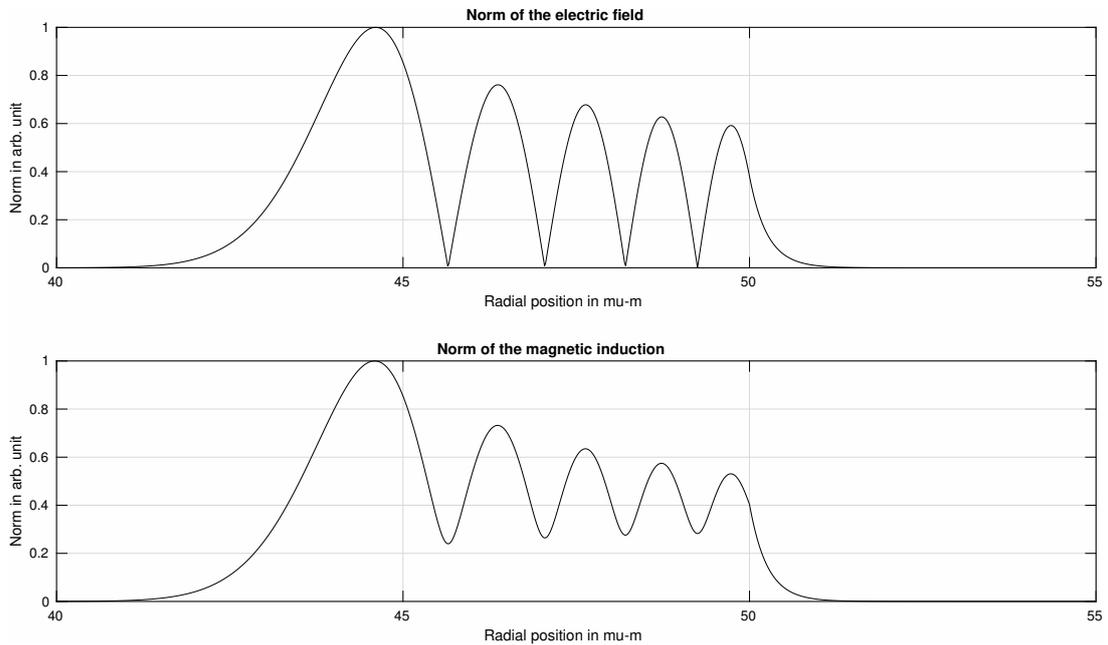


Figure 5: Radial behavior of the TE mode with polar index $\ell = 302$ and radial index $n = 5$ of a micro-sphere with radius $R = 50 \mu\text{m}$ and optical index $N = 1.5$.

The `pltmod` script also allows to draw the WGM field in an azimuthal plane $\varphi = cste$ as shown in Fig. 7 where we have represented the euclidean norms of the electric field and magnetic induction in the plane $\varphi = 0$ for the WGM with indexes $\ell = 302, m = 300, n = 1$ in the case of a spherical cavity with radius $R = 50 \mu\text{m}$ and optical index $N = 1.5$. Note that the norms of the electric field and magnetic induction are given in arbitrarily units since the WGM field is defined up to a multiplicative constant. Since a zoom in the area of interest in the MATLAB graphical window induces a loss in the image rendering, an expert mode is provided in the `pltmod` script (obtained by turning the variable `expert_mode` to the value 1 in the script). Fig. 7 was obtained using this feature with the following bound: $r \in [0.8 R, 1.1 R]$ and $\theta \in [0.8 \frac{\pi}{2}, 1.2 \frac{\pi}{2}]$. When this option is chosen it is possible to indicate the bounds of the area to plot (bounds for the polar angle θ and radial distance r). One can see in Fig. 7 that for the chosen data, we have $\ell - |m| + 1 = 3$ which is the number of intensity maxima in the polar direction \mathbf{e}_θ as stated on p. 3. Similarly, it is possible with the `pltmod` script also allows to draw the WGM field in an azimuthal plane $\theta = cste$.

```

>> pltmod
Micro-sphere radius [micro-m] R = 50
Optical index of the micro-sphere = 1.5
TE or TM mode : TE
Wavelength [nm] = 1502.024424
Mode number ell = 302
Mode number m = 300
Drawing options :
(A) 1D-plot in the radial direction
(B) 2D-plot in an azimuthal plane phi=cste
(C) 2D-plot in a polar plane theta=cste
Your choice (A/B/C) = B
Azimuthal angle [radian] : phi = 0
Minimum radial distance (% value of R) = 80
Maximal radial distance (% value of R) = 110
Minimum polar angle [radian] = pi/2-0.2*pi/2
Maximal polar angle [radian] = pi/2+0.2*pi/2

```

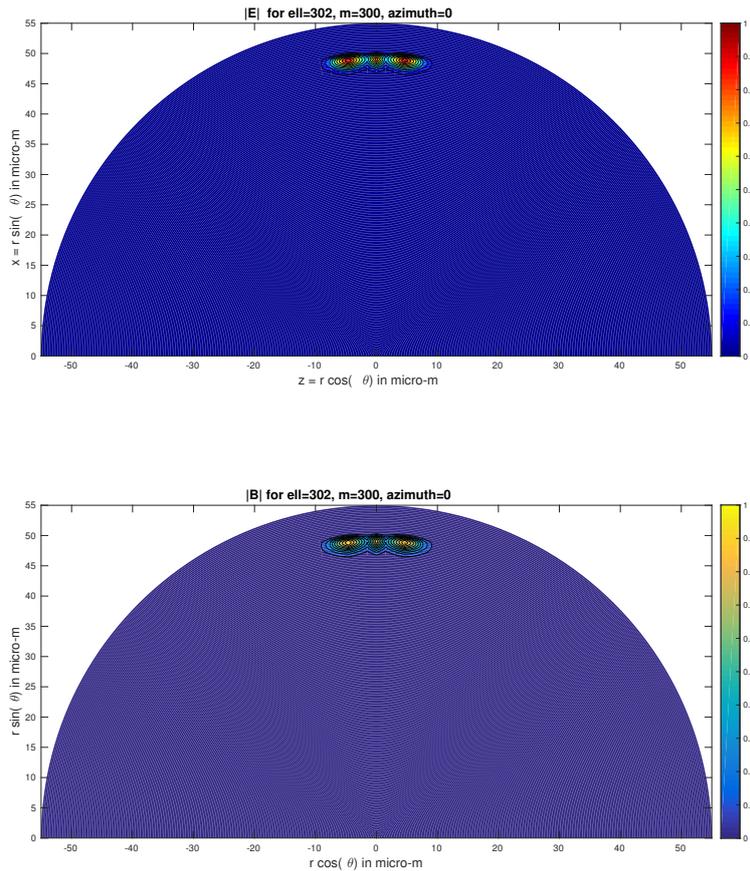


Figure 6: Euclidean norms of the electric field and magnetic induction in the plane $\varphi = 0$ for the WGM with indexes $\ell = 302, m = 300, n = 1$ in the case of a spherical cavity with radius $R = 50 \mu\text{m}$ and optical index $N = 1.5$.

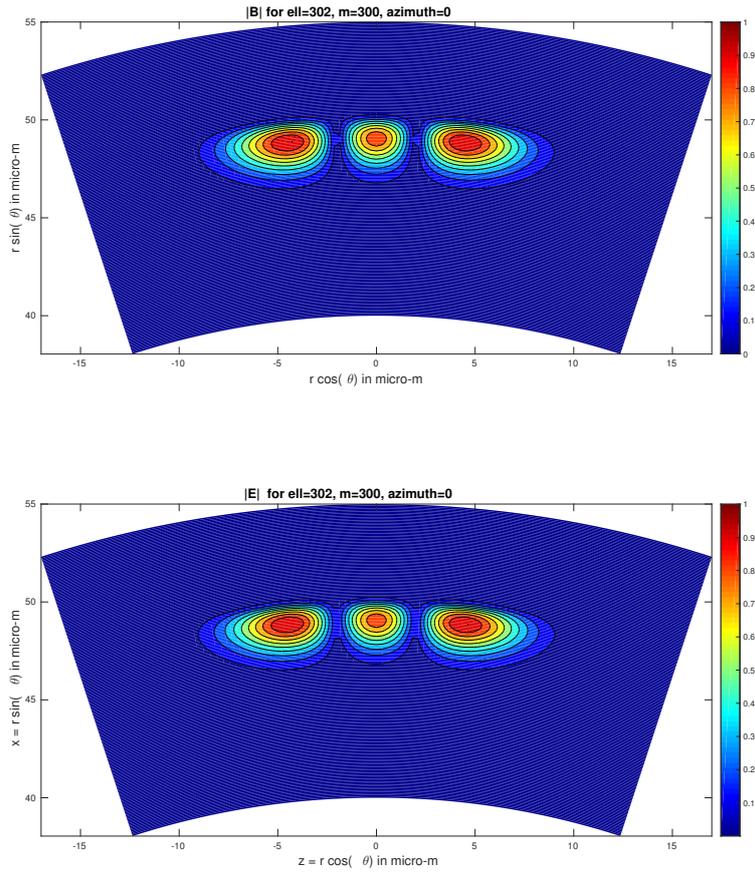


Figure 7: Euclidean norms of the electric field and magnetic induction in the plane $\varphi = 0$ for the WGM with indexes $\ell = 302, m = 300, n = 1$ in the case of a spherical cavity with radius $R = 50 \mu\text{m}$ and optical index $N = 1.5$.

With all the information at hand, we are now in position to compute the mode volume. For the dielectric micro-sphere with radius $R = 50 \mu\text{m}$ and optical index $N = 1.5$, let us consider the WGM characterized by the mode indexes $\ell = 302, m = \ell$ and $n = 1$ for which the resonance wavelength has been found to be $\lambda = 1502.024424 \text{ nm}$. Thanks to the `volmod` script in the `WGMODE` toolbox, we find that the volume of this WGM is $2259.6416 \mu\text{m}^3$ as detailed below.

```
>> volmod
Micro-sphere radius [micro-m] = 50
Optical index of the micro-sphere = 1.5
TE or TM mode ? (TE/TM) : TE
Wavelength [nm] = 1502.0244
Mode number ell = 302
Mode number m = 302
-----
Local minimum possible.

fminunc stopped because the size of the current step is less than
the default value of the step size tolerance.

<stopping criteria details>
```

```
-----  
Mode volume (in micron.m^3)= 2259.6416  
CPU time for mode volume computations = 1.58 sec.
```

Always for this particular WGM, using the `qfact` script, the quality factor is found to be $1.578 \cdot 10^{17}$. Note that this quality factor is not in accordance with the quality factor usually observed experimentally because radiative losses are much lower than intrinsic losses for such a micro-resonator. The tolerance values used to end iterations in the `fsolve` routine are set by default to 10^{-9} . These tolerance values can be modified using the expert mode by setting the `expert_mode` variable to the value 1 in the `qfact` script. Because solving equation (10) represents a stiff problem from a numerical point of view, the user should pay attention to the information returned by MATLAB `fsolve` routine to decide on the reliability of the quality factor value.

```
>> qfact  
Micro-sphere radius [micro-m] = 50  
Optical index of the micro-sphere = 1.5  
TE or TM mode ? (TE/TM) : TE  
Mode index ell = 302  
Approximated real value of the resonance wavelength [nm] = 1502  
-----  
Non-linear solver fsolve informations  
  
Equation solved.  
  
fsolve completed because the vector of function values is near zero  
as measured by the selected value of the function tolerance, and  
the problem appears regular as measured by the gradient.  
  
<stopping criteria details>  
  
-----  
Complex resonance wavelength for the mode in [nm] = 1502.024424398681  
-9.518987898596565e-15i  
Quality factor for the mode = 1.578e+17
```

Modifying the tolerance value of the `fsolve` solver using the expert mode can give information on the accuracy of the computed solution.

```
>> qfact  
Micro-sphere radius [micro-m] = 50  
Optical index of the micro-sphere = 1.5  
TE or TM mode ? (TE/TM) : TE  
Mode index ell = 302  
Approximated real value of the resonance wavelength [nm] = 1502  
Termination tolerance on the function value; TolFun = 1e-14  
Termination tolerance on the solution value; TolX = 1E-14  
-----  
Non-linear solver fsolve informations
```

```
Equation solved, inaccuracy possible.
```

```
The vector of function values is near zero, as measured by the selected value  
of the function tolerance. However, the last step was ineffective.
```

```
<stopping criteria details>
```

```
-----  
Complex resonance wavelength for the mode in [nm] = 1502.024424398681  
-9.518987898596565e-15i  
Quality factor for the mode = 1.578e+17
```

When comparing to the result returned by the Delves-Lyness method, see below, we obtain a very good agreement for the real part of the resonance wavelength but significantly different results for the imaginary part. One should note that the ratio of the imaginary part and the real part of the resonance is lower than the floating point accuracy and therefore the value returned for the quality factor should be considered with caution.

```
>> qfactn  
Micro-sphere radius [micro-m] = 50  
Optical index of the micro-sphere = 1.5  
TE or TM mode ? (TE/TM) : TE  
Mode index ell = 302  
Approximated real value of the resonance wavelength [nm] = 1502  
  
One root (wavelength resonance) of the modal equation located in the disk  
centered at 1502 nm with radius 1 nm  
  
Complex resonance wavelength for the mode in [nm] = 1502.024424398667  
-2.734045590480928e-13i  
Quality factor for the mode = 5.494e+15
```

5 A comprehensive test run under OCTAVE

In order to illustrate the use of the WGMODE toolbox under OCTAVE, we consider a micro-sphere of radius $25\ \mu\text{m}$ and optical index 1.453. We are interested in resonance conditions around a wavelength of 800 nm for TM modes. Results presented in this section were obtained with GNU Octave, version 4.0.0. First, we use the script entitled `ellres` to determine the solutions ℓ to the approximated modal equation (13) for wave numbers k and k_0 corresponding to a wavelength of 1500 nm and to a TM mode.

```
>> ellres  
Micro-sphere radius [micro-m] = 25  
Optical index of the micro-sphere = 1.453  
TE or TM mode ? (TE/TM) : TM  
Wavelength [nm] = 800
```

Polar mode indexes ell:

	1		273.289				6		238.780				11		214.990	
	2		264.217				7		233.567				12		210.780	
	3		256.809				8		228.618				13		206.723	
	4		250.277				9		223.891				14		202.823	
	5		244.319				10		219.355				15		199.010	

The expert mode can be activated by setting the variable `expert_mode` to 1 in the `ellres` program. It provides a plot of the modal function (22) the zero of which are the sought out solutions. The use of the `ellres` program in expert mode is illustrated below.

```
Micro-sphere radius [micro-m] = 25
Optical index of the micro-sphere = 1.453
TE or TM mode ? (TE/TM) : TM
Wavelength [nm] = 800
Interval of interest for the mode indices search : [0,300]
```

Polar mode indexes ell:

	1		273.289				9		223.891				17		188.954				25		117.581	
	2		264.217				10		219.355				18		183.882				26		101.623	
	3		256.809				11		214.990				19		177.135				27		83.372	
	4		250.277				12		210.780				20		169.978				28		82.016	
	5		244.319				13		206.723				21		161.857				29		81.623	
	6		238.780				14		202.823				22		152.745				30		57.124	
	7		233.567				15		199.010				23		142.836				31		56.364	
	8		228.618				16		195.030				24		131.274				32		55.179	

The OCTAVE graphic windows opens with the representation of the modal function F_λ defined in (22) for $\lambda = 800\text{nm}$ over the interval $[0, 300]$, see Fig. 8.

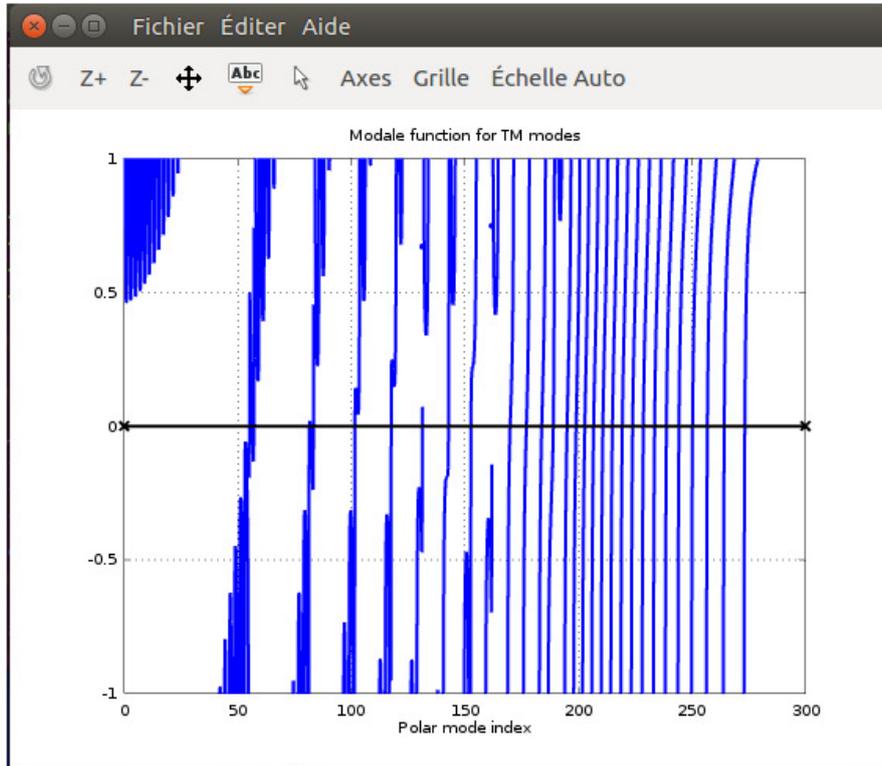


Figure 8: Modal function F_λ defined in (22) for $\lambda = 800$ nm over the interval $[0, 300]$.

As can be seen above, the mode indexes ℓ obtained as solutions to the modal equation (10) are not integers. Thus, we have to round up the values to the nearest integer. But doing so, the couple (λ, ℓ) doesn't anymore satisfies the modal equation. For each rounded values for ℓ , we have to compute the resonance wavelength by solving once again the modal equation. This time, ℓ is fixed and we look for λ . Computation is achieved with the MATLAB script named `wvlres`. As an example, we consider the first value for ℓ (264.217), rounded to 264.

```
>> wvlres
Micro-sphere radius [micro-m] = 25
Optical index of the micro-sphere = 1.453
TE or TM mode ? (TE/TM) : TM
Polar mode index ell = 264

Wavelength interval of interest found [nm] = [594.884 , 865.034]

Radial mode number and resonance wavelength [nm]:

| 1 | 827.336260 |           | 8 | 706.231082 | | | |
| 2 | 800.625109 |           | 9 | 694.818246 |           | 15 | 638.102578 |
| 3 | 779.659735 |           | 10 | 684.086562 |           | 16 | 630.111569 |
| 4 | 761.776557 |           | 11 | 673.947165 |           | 17 | 622.456282 |
| 5 | 745.938682 |           | 12 | 664.330083 |           | 18 | 615.122231 |
| 6 | 731.603396 |           | 13 | 655.179180 |           | 19 | 608.073387 |
| 7 | 718.440811 |           | 14 | 646.448935 |           | 20 | 601.206674 |
```

An expert mode can be activated by setting the variable `expert_mode` to 1 in the `wvlres`

program. It allows to compare the resonance wavelengths to the one obtained from the Eikonale approach, see e.g. [3, 9], which basically relies on asymptotic expansion for Bessel's functions of large order. It also provides a plot of the modal function F_ℓ defined by (23) the zero of which are the sought out solutions.

```
>> wvlres
Micro-sphere radius [micro-m] = 25
Optical index of the micro-sphere = 1.453
TE or TM mode ? (TE/TM) : TM
Polar mode index ell = 264
Interval of interest for the wavelength search [nm]: [700 900]

Radial mode number and resonance wavelength [nm]:

| 1 | 827.336260 |
| 2 | 800.625107 |
| 3 | 779.659734 |
| 4 | 761.776557 |
| 5 | 745.938679 |
| 6 | 731.603394 |
| 7 | 718.440808 |
| 8 | 706.231082 |

Compare results to the Eikonale equation ? [y/n] : y

Radial mode number and resonance wavelength from the Eikonale equation [nm]:

| 1 | 827.939140 |
| 2 | 801.833970 |
| 3 | 781.749632 |
| 4 | 764.835172 |
| 5 | 750.006578 |
| 6 | 736.699653 |
| 7 | 724.572252 |
| 8 | 713.396692 |
```

The OCTAVE graphic windows opens with the representation of the modal function F_ℓ defined in (23) for $\ell = 264$ and $\lambda \in [700, 900]$ see Fig. 9.

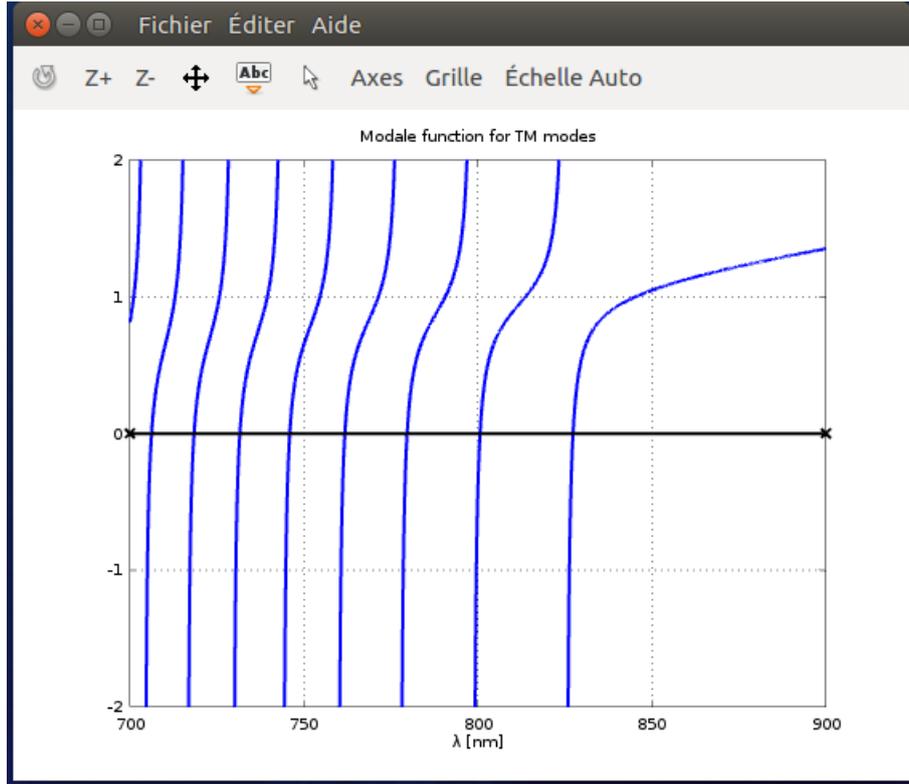


Figure 9: Modal function F_ℓ defined in (23) for $\ell = 264$ and $\lambda \in [700; 900]$.

The `pltmod` script of the `WGMODE` toolbox that was developed to draw the WGM field. Three different plots of the euclidean norm of the electric field $\|\mathbf{E}(r, \theta, \varphi)\|$ and magnetic induction $\|\mathbf{B}(r, \theta, \varphi)\|$ are proposed. They correspond to a 1D-plot in the radial direction, to a 2D-plot in an azimuthal plane $\varphi = \text{cste}$ and to a 2D-plot in a polar plane $\theta = \text{cste}$. Note that the `pltmod` script does not give a satisfactory results under OCTAVE due to an excessive computational time in the evaluation of the WGM field at the grid points (call to the `modefield` function of the `WGMODE` toolbox).

```
>> pltmod
Micro-sphere radius [micro-m] R = 25
Optical index of the micro-sphere = 1.453
TE or TM mode : TM
Wavelength [nm] = 827.336260
Mode number ell = 264
Mode number m = 262
Drawing options :
(A) 1D-plot in the radial direction
(B) 2D-plot in an azimuthal plane phi=cste
(C) 2D-plot in a polar plane theta=cste
Your choice (A/B/C) = A
Minimum radial distance (% value of R) = 50
Maximal radial distance (% value of R) = 200
```

We have depicted in Fig. 10 the radial variation of the electric field and magnetic induction for $(\theta, \varphi) = (\frac{\pi}{2}, 0)$ corresponding to the TM mode with polar index $\ell = 264$ and radial index $n = 1$. Note that the unit is arbitrary since the mode field is defined up to a multiplicative

constant. One can clearly see in the figure one maxima in the radial direction as expected for a mode with radial index $n = 1$.

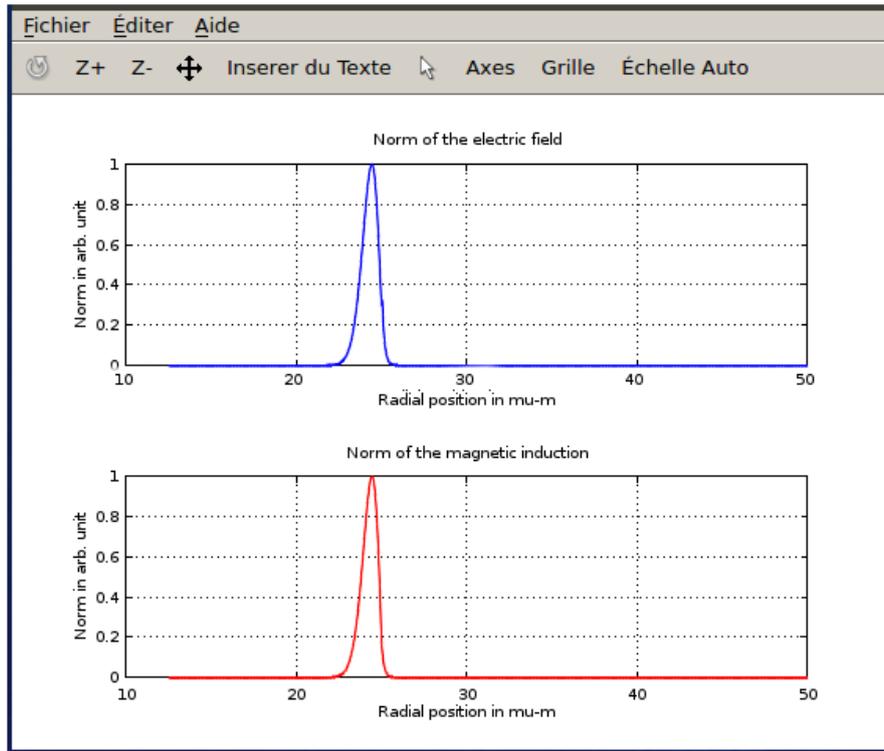


Figure 10: Radial behavior of the TM mode with polar index $\ell = 264$ and radial index $n = 1$ of a micro-sphere with radius $R = 25 \mu\text{m}$ and optical index $N = 1.453$.

Let us now proceed to the computation of the TM mode volume characterized by the mode indexes $\ell = 264, m = 262$ and $n = 1$ of the dielectric micro-sphere with radius $R = 50 \mu\text{m}$ and optical index $N = 1.453$.

```
>> volmod
Micro-sphere radius [micro-m] = 25
Optical index of the micro-sphere = 1.453
TE or TM mode ? (TE/TM) : TM
Wavelength [nm] = 827.336260
Mode number ell = 264
Mode number m = 262

No optimization toolbox found
Maximization by values comparison launched
Mode volume (in micron.m^3)= 513.76
CPU time for mode volume computations = 1.567e+04 sec.
```

Note that the `volmod` script under OCTAVE provide the mode volume after a very long computational time.

Always for this particular WGM, using the `qfact` script, the quality factor is find to be $1.578 \cdot 10^{17}$. Note that this quality factor is not in accordance with the quality factor usually

observed experimentally because radiative losses are much lower than intrinsic losses for such a micro-resonator. The tolerance values used to end iterations in the `fsolve` routine are set by default to 10^{-9} . These tolerance values can be modified using the expert mode by setting the `expert_mode` variable to the value 1 in the `qfact` script. Because solving equation (10) represents a stiff problem from a numerical point of view, the user should pay attention to the information returned by MATLAB `fsolve` routine to decide on the reliability of the quality factor value.

```
>> qfact
Micro-sphere radius [micro-m] = 25
Optical index of the micro-sphere = 1.453
TE or TM mode ? (TE/TM) : TM
Mode index ell = 264
Approximated real value of the resonance wavelength [nm] = 827
-----
Non-linear solver fsolve informations
-----
Complex resonance wavelength for the mode in [nm] = 827.3362584354486
+8.973945396233738e-14i
Quality factor for the mode = 9.219e+15
```

When comparing to the result returned by the Delves-Lyess method for the computation of the quality factor using the script `qfactn`, we obtain a very good agreement for the real part of the resonance wavelength but significantly different results for the imaginary part. One should note that the ratio of the imaginary part and the real part of the resonance is lower than the floating point accuracy and therefore the value returned for the quality factor should be considered with caution.

```
>> qfactn
Micro-sphere radius [micro-m] = 25
Optical index of the micro-sphere = 1.453
TE or TM mode ? (TE/TM) : TM
Mode index ell = 264
Approximated real value of the resonance wavelength [nm] = 827

One root (wavelength resonance) of the modal equation located
in the disk centered at 827 nm with radius 1 nm

Complex resonance wavelength for the mode in [nm] = 827.3362584354487
-4.254327798283179e-16i
Quality factor for the mode = 1.945e+18
```

6 Additional comments

In the normal mode for using the `WGMODE` toolbox (obtained by setting to zero the variable `expert_mode` defined on the first lines of the scripts of the `WGMODE` toolbox), relation (20) is used in the script `ellres` to have bounds for the interval where the solutions ℓ to equation (13) have to be sought out. Similarly, relation (21) is used in the script `ellres` to have bounds for the interval where the solutions k_0 to equation (13) have to be sought out. These bounds

have been established in [9, p. 25] for WGMs in ordinary spherical cavities. It may happen that for some reason (e.g. spherical cavity with unusual characteristics), no solution is found in the given interval. Using the expert mode, the user can overcome this issue by providing his own bounds as illustrated below.

Example under the normal mode. (We first check the value of variable `expert_mode` in file `ellres.m`.)

```
>> !more wvlres.m
%WVLRES COMPUTES THE WAVELENGTH AT RESONANCE
%   WVLRES computes, for a given mode index, the values of the wavelength
%   for which a resonance occurs

clear
close all
expert_mode=0; % set to 1 for using the programm in expert mode

>> wvlres
Micro-sphere radius [micro-m] = 5
Optical index of the micro-sphere = 1.2
Polar mode index ell = 5
TE or TM mode ? (TE/TM) : TE

Wavelength intervalle of interest found [nm] = [7868.8473 , 10213.9819]
No solution found ...
```

The same example under the expert mode. The variable `expert_mode` in the file `ellres.m` must be set to the value 1. We check its value before running the script.

```
>> !more wvlres.m
%WVLRES COMPUTES THE WAVELENGTH AT RESONANCE
%   WVLRES computes, for a given mode index, the values of the wavelength
%   for which a resonance occurs

clear
close all
expert_mode=1; % set to 1 for using the programm in expert mode

>> wvlres
Micro-sphere radius [micro-m] = 5
Optical index of the micro-sphere = 1.2
TE or TM mode ? (TE/TM) : TE
Polar mode index ell = 5
Interval of interest for the wavelength search [nm]: [0,1500]

Radial mode number and resonance wavelength [nm]:

|  1 | 1329.243684 |
|  2 | 799.753111 |
|  3 | 571.385200 |
|  4 | 63.492062 |
|  5 | 59.701492 |
|  6 | 56.338029 |
|  7 | 53.333334 |
```

8	51.949475
9	47.058824
10	42.105263
11	21.544059
12	11.267605
13	6.400000
14	5.281225

Compare results to the Eikonale equation ? [y/n] : n

References

- [1] J. Stratton, *Electromagnetic Theory*, Wiley, 2007.
- [2] A. N. Oraevsky, Review: Whispering-gallery waves, *Quantum Electronics* 32 (2002) 377–400. doi:10.1070/QE2002v032n05ABEH002205.
- [3] G. C. Righini, Y. Dumeige, P. Féron, M. Ferrari, G. N. Conti, D. Ristic, S. Soria, Whispering gallery mode microresonators: Fundamentals and applications, *Rivista del Nuovo Cimento* 34 (7) (2011) 435–488. doi:10.1393/ncr/i2011-10067-2.
- [4] F. Olver, D. Lozier, R. Boisvert, C. Clark, *NIST Handbook of Mathematical Functions*, Cambridge University Press, 2010.
- [5] M. Abramowitz, I. A. Stegun, *Handbook of Mathematical Functions: with Formulas, Graphs, and Mathematical Tables*, Dover Publications, 1965.
- [6] K. Atkinson, W. Han, *Spherical Harmonics and Approximations on the Unit Sphere: An Introduction*, Lecture Notes in Mathematics, Springer, 2012.
- [7] R. Talebi, K. Abbasian, A. Rostami, Analytical modeling of quality factor for shell type microsphere resonators, *Progress In Electromagnetics Research B* 30 (2011) 293–311. doi:10.2528/PIERB11040303.
- [8] M. Borselli, T. Johnson, O. Painter, Beyond the rayleigh scattering limit in high-Q silicon microdisks: Theory and experiment, *Opt. Express* 13 (5) (2005) 1515–1530. doi:10.1364/OPEX.13.001515.
- [9] F. Treussart, Étude expérimentale de l’effet laser dans des micro-sphères de silice dopées avec des ions néodyme, Ph.D. thesis, Université Pierre et Marie Curie, Paris, France (1997).
- [10] T.J.A.Kippenberg, Nonlinear optics in ultra-high-Q whispering-gallery optical microcavities, Ph.D. thesis, California Institute of Technology, Pasadena, California, USA (2004).
- [11] E. A. Muljarov, W. Langbein, Exact mode volume and purcell factor of open optical systems, *Phys. Rev. B* 94 (2016) 235438. doi:10.1103/PhysRevB.94.235438.
- [12] J. D. Jackson, *Classical Electrodynamics*, 3rd Edition, Wiley, 1998.
- [13] L. M. Delves, J. N. Lyness, A numerical method for locating the zeros of an analytic function, *Math. Comp.* 21 (1967) 543–560. doi:10.2307/2004999.

- [14] N. I. Ioakimidis, Quadrature methods for the determination of zeros of transcendental functions - a review, in: P. Keast, G. Fairweather (Eds.), Numerical Integration: Recent Developments, Software and Applications, Springer Netherlands, Dordrecht, 1987, pp. 61–82. doi:10.1007/978-94-009-3889-2_5.