Computer Physics Communications 185 (2014) 1200–1206

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Numerical simulation of the whispering gallery modes in prolate spheroids

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ARTICLE INFO

Article history:
Received 24 October 2013
Received in revised form
25 November 2013
Accepted 8 December 2013
Available online 16 December 2013

Keywords:
Morphology dependent resonances
'Whispering gallery' mode
Multi-parameter spectral problems
Prüfer angle
High order finite difference schemes

ABSTRACT

In this paper, we discuss the progress in the numerical simulation of the so-called 'whispering gallery' modes (WGMs) occurring inside a prolate spheroidal cavity. These modes are mainly concentrated in a narrow domain along the equatorial line of a spheroid and they are famous because of their extremely high quality factor. The scalar Helmholtz equation provides a sufficient accuracy for WGM simulation and (in a contrary to its vector version) is separable in spheroidal coordinates. However, the numerical simulation of 'whispering gallery' phenomena is not straightforward. The separation of variables yields two spheroidal wave ordinary differential equations (ODEs), first only depending on the angular, second on the radial coordinate. Though separated, these equations remain coupled through the separation constant and the eigenfrequency, so that together with the boundary conditions they form a singular self-adjoint two-parameter Sturm–Liouville problem.

We discuss an efficient and reliable technique for the numerical solution of this problem which enables calculation of highly localized WGMs inside a spheroid. The presented approach is also applicable to other separable geometries. We illustrate the performance of the method by means of numerical experiments.

1. Introduction and preliminaries

WGM resonators are of growing interest due to their exceptional properties, like an extremely high quality factor, or Q-factor, which indicates the rate of energy loss relative to the stored energy of the resonator. WGM resonators are encountered in numerous applications in science and industry, in such fields as optics and photonics [1].

An overview of the state of research on WGMs is provided in the recent publications [2,3]. Although the theory of WGMs is well developed, the numerical simulation of these phenomena is not an easy task. The only exceptions are spherical and cylindrical resonators, for which precise calculations of eigenmodes, radiative losses, and field distributions are available [3,4].

In the recent years, numerous attempts have been made to perform calculations of WGMs inside resonators of a non-spherical shape. In [5,6] a direct finite-element simulation of WGMs inside ellipsoidal and toroidal resonators was presented. However, the limitations inherent in the finite-element approach do not allow to accurately calculate extremely highly localized oscillations.

If the shape of a resonator allows separation of variables in the modeling equation, this simplifies essentially both the analytical and numerical analysis. Unfortunately, the above mentioned cases of a sphere and a cylinder expire the variety of separable geometries for the Helmholtz vector equation. However, WGMs inside spheroids may be still well modeled using the scalar Helmholtz equation which is separable in spheroidal coordinates [7,8]. A very detailed analysis of WGMs in spheroidal cavities given in [7] can be considered as a starting point of the present publication.

In the sequel, we report on a progress which we could achieve in the numerical simulation of WGMs occurring inside a prolate spheroid. Following the considerations in [7], the WGM phenomenon is simulated using the scalar Helmholtz equation. Either Dirichlet or Neumann boundary conditions are imposed on the boundary surface of the resonator and variables are separated in the prolate spheroidal coordinates. In the next section, we shall give an exact formulation of the problem arising thereby.

After the separation of variables, we obtain a system of ODEs (prolate spheroidal wave equations), depending on either angular or radial coordinate. These equations remain coupled via the separation constant and the eigenfrequency. Together with the

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0010-4655/$ – see front matter
http://dx.doi.org/10.1016/j.cpc.2013.12.012

boundary conditions they result in a singular self-adjoint two-parameter Sturm–Liouville problem.

The general theory of multi-parameter spectral problems is now well-developed [9–11]. Applied to the problem at hand, it guarantees the existence of a two-parameter eigenvalue and an associated two-component eigenfunction for any multi-index $(l,\ k)$, i.e. a pair of two non-negative integers $l,\ k$, indicating the number of oscillations of the eigenfunction components.

The multi-index $(l,\ k)$ and the azimuthal number m provide a very convenient opportunity to single out WGMs from the whole variety of oscillations inside a spheroid. WGMs are modes corresponding to small indices l and k ($l, k \sim 0$–3) and extra large azimuthal numbers $m \sim 1000$–10000.

Even in the simplest cases numerical solution of a singular two-parameter Sturm–Liouville problem requires special care. First we transfer those boundary conditions which are necessary and sufficient for the solution to stay bounded, from the singular points to the close regular points, see [12,13]. In the second step, we apply to such a 'regularized problem' a properly modified algorithm developed in [14] for the evaluation of the angular ellipsoidal (Lamé) wave functions. This algorithm is based on the WKB asymptotics[1] of the bounded solutions of the prolate spheroidal wave equations, i.e. on the related Prüfer angles, and it allows calculation of even extremely rapidly oscillating solutions. Yet, in the WGMs case, the rapidly oscillating angular azimuthal component is known *a priori*, while the evaluated components practically do not oscillate: they vanish on a large part of their domain and change sharply only in a very narrow subinterval. This restricts the computational accuracy of the Prüfer angles in case of the low-oscillatory components, and the calculations may become unstable. In spite of that, the Prüfer angle can be used to localize the desired eigenvalue and to provide a very accurate initial guess for a subsequent calculation of the desired WGMs using the Newton's iteration. The latter is carried out after the discretization of the spheroidal wave equations based on the high-order difference schemes and provide very accurate approximation for both, the WGM eigenfrequency and the associated solution of the scalar Helmholtz equation.

2. Prolate spheroidal coordinates and prolate spheroidal wave functions

In this section we collect the most important facts concerning the problem setting. For more details see [7,16] and the literature therein.

Prolate spheroidal coordinates are introduced via their relations to the conventional Cartesian coordinates,

$$x = \frac{d}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\cos\varphi,$$
$$y = \frac{d}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\sin\varphi, \qquad z = \frac{d}{2}\xi\eta,$$

where $\varphi \in [0,\ 2\pi)$ is the azimuthal angle, while $\eta \in (-1, 1)$ and $\xi \in (1, \infty)$ play the roles of inclination and radius, respectively. The corresponding coordinate surfaces are confocal two-sheeted hyperboloids of revolution and prolate spheroids, with d being the distance between the foci.

The eigenvalue problem for the Laplace operator defined on the domain bounded by a spheroid $\xi = \xi_s$,

$$-\Delta W(\mathbf{r}) = \hat{k}^2 W(\mathbf{r}), \qquad \mathbf{r} = (\varphi, \eta, \xi), \quad \xi < \xi_s,$$

is separable in spheroidal coordinates, provided that either Dirichlet or Neumann boundary conditions are imposed. Any particular solution of the problem is represented as a product of its angular, radial and azimuthal part,

$$W(\mathbf{r}) = S(\eta)R(\xi)\exp(\pm i\,m\,\varphi), \quad m = 0, 1, \ldots.$$

Functions $S(\eta)$ and $R(\xi)$ are bounded solutions of the angular and radial prolate spheroidal wave equations, respectively,

$$\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta}S + \left[\lambda + c^2(1-\eta^2) - \frac{m^2}{1-\eta^2}\right]S = 0,$$
$$-1 < \eta < 1, \tag{1}$$

$$\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi}R + \left[c^2(\xi^2-1) - \lambda - \frac{m^2}{\xi^2-1}\right]R = 0,$$
$$1 < \xi < \xi_s. \tag{2}$$

Here λ denotes the separation constant, and $c = \hat{k}\,d/2$.

Note that the differential operator in (1) exhibits two singular points at $\eta = \pm 1$, while Eq. (2) has a singular point $\xi = 1$.

Due to the symmetry of the problem, one can consider (1) on the half-interval $[0, 1)$, requiring the angular function $S(\eta)$ to be either odd or even, and satisfying respectively, the following initial condition:

$$S(0) = 0, \qquad S'(0) = 0. \tag{3}$$

The boundary condition on the surface of the spheroid implies for the radial function $R(\xi)$ that either one of the following terminal conditions holds:

$$R(\xi_s) = 0, \qquad R'(\xi_s) = 0. \tag{4}$$

Solutions of the system (1), (2) bounded at singular points $\eta = 1$ and $\xi = 1$ satisfy the boundary conditions (3), (4) not for all λ and c^2. If for a pair (λ, c^2) there exists a bounded non-trivial solution to each of the problems (1), (3) and (2), (4), such a pair is called a two-parameter eigenvalue of the system. Hereafter, we specify eigenvalues (λ, c^2) with a multi-index (l, k), in which the integers l and k count the numbers of internal zeros of the associated angular and radial functions, $S_{lk}(\eta)$ and $R_{lk}(\xi)$, inside the intervals $(-1, 1)$ and $(1, \xi_s)$. Note that the parity of the index l defines the parity of the angular function S_{lk}.

In addition, functions $S_{lk}(\eta)$ and $R_{lk}(\xi)$ are normalized by

$$\int_{-1}^{1} S_{lk}^2(\eta)\,d\eta = 1, \qquad \int_{1}^{\xi_s} R_{lk}^2(\xi)\,d\xi = 1. \tag{5}$$

In the sequel, the multi-index $(l,\ k)$ as well as the azimuthal number m are fixed, and $m > 0$. Although the case $m = 0$ does not cause any additional difficulty, it should be considered separately. Here, we omit this case, since it plays no role in the simulation of the 'whispering gallery' phenomenon.

3. Boundary conditions transferred to a regular point

The numerical technique presented below is not applicable to singular boundary value problems, therefore we shall formulate an equivalent regular boundary value problem on the domain $(0,\ 1-\delta_\eta) \times (1+\delta_\xi,\ \xi_s)$ with $\delta_\eta > 0$ and $\delta_\xi > 0$ chosen to exclude singular points from the integration interval.

Let us first consider Eq. (1). Here, the singularity at the point $\eta = 1$ is indeed regular [17]. Unless $m = 0$, any bounded solution of (1) behaves as [16],

$$S(\eta) \sim (1-\eta^2)^{m/2}, \quad \eta \to 1-.$$

For (2), the singularity at the point $\xi = 1$ is again regular; for a solution bounded at $\xi = 1$ the following asymptotic holds:

$$R(\xi) \sim (\xi^2-1)^{m/2}, \quad \xi \to 1+.$$

[1] An asymptotic method introduced by G. Wentzel, H. Kramers, L. Brillouin, and H. Jeffreys to obtain approximate solutions of Schrödinger equation. For a detailed historical account and literature see e.g. [15].