Chaos-Free Mathematical Framework for Linear Optical Modelling of Microcavities and Microlasers

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ABSTRACT
We review basic facts from the theory of linear Maxwellian boundary-value problems for dielectric open resonators that establish the classical mathematical framework for the accurate modelling of microcavities. We discuss how a small modification of this theory delivers modal thresholds in addition to lasing frequencies.
Keywords: microcavity laser, integral equations, eigenvalue problem, Q-factor, linear threshold.

1. INTRODUCTION

Today's trends in microcavity lasers research can be seen in smoothing the cavity rim, optimising the shape of the pumped area, looking for optimal cavity shapes, integrating microdisks with optical fibres, building arrays of microdisks, and shrinking the active region to a few individual quantum dots (QDs). Besides of the shown in Fig. 1 air-clad on-pedestal versions, these structures can be also manufactured as on-low-index-substrate ones.

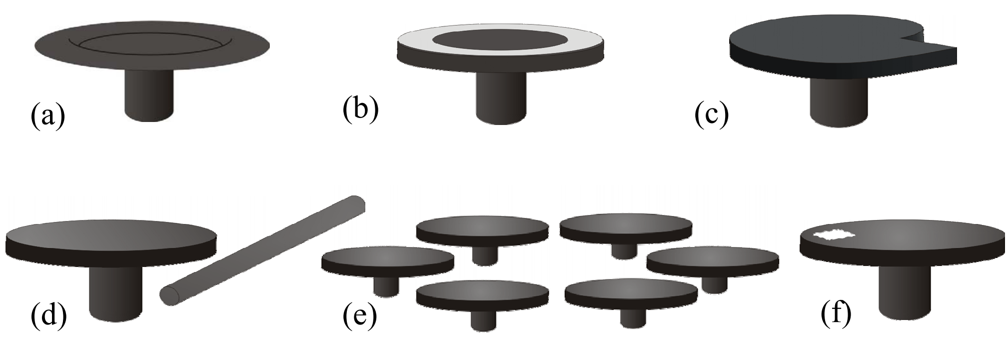

Figure. 1. Some of novel designs of microdisk lasers: (a) disk with a rounded rim, (b) disk with a ring-shape active region, (c) disk having "spiral"-shape cavity, (d) disk loaded with a tapered optical fibre, (e) cyclic photonic molecule of disks, and (f) disk with single quantum-dot active region.

For comprehensive modelling of the microcavity laser, several fundamental mechanisms should be accounted for, such as transport of carriers, stimulated emission, heating, and optical field confinement. Nonlinear effects link them together and limit the output power. However, a reasonable reduction of complexity can be achieved within a linear optical problem neglecting all non-electromagnetic phenomena and viewing the optical modes as solutions to Maxwell equations. Traditionally, this simulation neglects the pedestal, which is assumed to have no effect on the working whispering-gallery (WG) modes, and nonuniformity in the z direction (the z-axis being the disk rotation axis), due to the very small thickness of active-region layers. It also uses a reduction of dimensionality from 3-D to 2-D in the disk plane, with the effective-index method. Further, the goal is finding the frequencies and Q-factors of the natural modes of the *passive cavities* [1].

2. COMPLEX-FREQUENCY EIGENVALUE PROBLEMS: DISCRETENESS AND INCOMPLETENESS OF MODES

2.1 3-D formulation

For simplicity, assume that a microcavity has finite volume V bounded with a smooth surface S, and the host medium is free space so that the refractive index is a constant α inside S and 1 outside. The full frequency eigenvalue problem implies that we seek the natural frequencies k (normalized by the light velocity, c) generating nontrivial fields $\{\vec{E},\vec{H}\}e^{-ikct}$, which solve, off the cavity surface S, the set of *homogeneous time-harmonic Maxwell equations*. Additionally, *transmission conditions* are requested on S: tangential field components must be continuous. Further, the electromagnetic energy must be locally integrable to prevent source-like field singularities, and, eventually, we must also include a certain *condition at infinity* ($R \to \infty$).

It plays an important role and in 3-D has the form of the Silver-Muller radiation condition [2], which provides for the outgoing spherical-wave behavior and, in addition, eliminates non-transverse field components at infinity. All above mentioned conditions are "inherited" from the more general wave-scattering problem (they guarantee the solution uniquesness there, for real *k*) and form an eigenvalue boundary-value problem (BVP).

It is possible to establish important general properties of the eigenfrequencies even before solving the formulated BVP. The Poynting theorem, applied to an eigenfunction $\{\vec{E},\vec{H}\}$ and its complex conjugate, leads to the conclusion that, independently of the geometry of the open resonator, real-valued eigenfrequencies do not exist; therefore it is necessary to admit complex values of *k*. Then similar treatment leads to the conclusion that the eigenvalues can be located only in the lower halfplane of the *k*-plane; i.e., each of them has $\operatorname{Im} k < 0$, for the selected time dependence. This corresponds to the damping in time due to radiation losses; by the same reason field functions $\{\vec{E},\vec{H}\}$ diverge at infinity as $O(e^{-\operatorname{Im} kR}/R)$. In this sense, the eigenfrequencies of an open cavity are *generalized eigenvalues* generating *generalized eigenfunctions*. Direct check shows that they come in pairs: if *k* is eigenvalue, so is $-k^*$; this is a consequence of the time invariance in harmonic problems.

Further, our BVP is equivalently reducible to a set of two coupled boundary IEs of the second kind with smooth or integrable kernels analytic on the complex *k*–plane (so-called Muller IEs) [2, 3]. Therefore, they can be viewed as a canonical Fredholm-type operator equation, and hence the Fredholm theorems generalized for operators are valid [4,5]. They tell that the eigenfrequencies form a *discrete* set in any bounded domain on the *k*–plane; they have no finite accumulation points; they can appear or disappear only at infinity; and they have finite multiplicity. Therefore, one can number them with an index, say *s*, and be sure that no lines or lacunas filled with eigenfrequencies can be hit when looking for k_s numerically. Even more important is that each k_s is a piece-continuous or piece-analytic function of geometry and refractive index, and these properties can be lost only if one or more eigenvalues coalesce. The eigenfunction $\{\vec{E}_s,\vec{H}_s\}=\{\vec{E}(k_s),\vec{H}(k_s)\}$ gives the field function, and the entity of eigenfrequency and eigenfunction is considered as a *mode.* Their quality factors are defined as $Q_s = |\operatorname{Re} k_s / 2\operatorname{Im} k_s| > 0$. As mentioned, the eigenfrequencies may coincide that is called *modal degeneracy*. If the degeneracy is caused by the symmetry of the cavity (geometrical degeneracy) then the modal fields are orthogonal to each other as belonging to different symmetry classes; if it is caused by the coalescence of the eigenfrequencies of the same symmetry class when varying some parameter (algebraic degeneracy), then, besides of eigenfunction, a finite chain of *associated functions* appear; all together such functions are called *root functions*.

Unfortunately, it looks like the complex-valued nature of eigenfrequencies, albeit necessary for the physical adequacy, makes them inapplicable as the solution building blocks in the scattering BVP when the frequency of the incident wave, *k*, is real-valued. Indeed, orthogonality between the eigenfunctions of the same class can be established only at the expense of introducing a super-exponentially decaying weight to compensate for their spatial divergence [6]. This, together with the absence of *completeness* for the set of generalized modes of an open cavity, prevents from using such modes as a functional basis in the scattering problems.

2.2 Effective-index reduction to the 2-D problem for a thin cavity

Reduction of dimensionality of a microcavity BVP from 3-D to 2-D implies that the cavity thickness is a fraction of both its diameter and the wavelength. In its core one finds the assumption that the field dependences on the normal (z) and in-plane (r,φ) coordinates are separable. In fact, this is incorrect because neither the boundary conditions on the 3-D disk surface *S*, nor the radiation condition at $R\to\infty$, are separable. However, this leads to decoupled differential equations for the functions of *z* and (r,φ). The first of them brings a set of dispersion equations for the "effective index" as a normalized wavenumber of the natural guided wave on an infinite dielectric slab of the same thickness as disk. For the in-plane fields, $U(x,y)=E_z$ or H_z, one obtains independent BVPs for the 2-D Helmholtz equation with the squared effective refractive index in coefficient. The transmission-type boundary conditions now depend on the polarization; 2-D power finiteness and radiation conditions should be added. Note also that the effective index is a function of frequency and has a discrete set of values corresponding to different slab waves. Generally speaking, a 3-D problem is not equivalent mathematically to the "sum" of 1-D and 2-D problems. Nevertheless, it is well known that the results obtained with the effective-index method are often more accurate than might be expected.

In 2-D, equivalent to BVP IEs lead to the same conclusions about the discreteness, finite multiplicity, and continuous dependence of eigenfrequencies on parameters as in 3-D case. However, they are now located not on the complex *k*-plane but on the Riemann surface of the function $\operatorname{Ln} k$. This is because in 2-D the Green's function is the Hankel function, $H_0^{(1)}(k|\bar{r}-\bar{r}'|)$, known to have a logarithmic branching point if the argument turns zero. Incompleteness of eigenfreuencies is still more obvious in 2-D as on the Riemann surface of $\operatorname{Ln} k$ it is impossible to draw a closed contour around the origin; therefore Mittag-Leffler theorem is not applicable.

2.3 Where hides the chaos?

It should be emphasised that the mathematical theory of linear electromagnetic BVPs and equivalent to them IEs gives no ground for classification of non-circular dielectric cavities as stable, unstable and chaotic. Any passive open resonator possesses a discrete albeit infinite set of complex-valued natural frequencies. Each eigenvalue k_s generates a unique eigenfunction – this is the modal field characterised by two corresponding vector-functions, $\vec{E}_s$ and $\vec{H}_s$ (in 3-D) or one scalar function U_s (in 2-D). In this sense, all WG and "bow-tie" or "scar" modes are perfectly stable although differ in the values of their frequencies and Q-factors.

In linear problem, "chaos" appears only when we try to simplify the task and superimpose a ray-tracing approximation on the intrinsically wave-like solutions of the Maxwell equations [7]. Mathematically, there is a well-established understanding that both Maxwell and Helmholtz equations have what is called an elliptic behaviour. This means that the whole modal field must be found simultaneously in accordance with the boundary conditions on the entire surface of the cavity. In contrast, the rays emerge as solutions to the eikonal equation, which is an extreme form of the parabolic equation that, in its turn, approximates exact ones only for the field behaving as a locally–plane wave. Parabolic equations, indeed, allow a huge computational simplification as they can be solved step-by-step downstream from a start point. For the rays this simplification goes even further and reduces to the Snell law of the specular reflection from the boundary of cavity. This is where the chaos emerges in the form of chaotic trajectories of rays. Therefore the chaos is the cost of pleasure – in the same manner as the branching of the habitat of complex eigenfrequencies is the cost of switching from the accurate 3-D to an approximate 2-D BVP for the natural modes of open cavity.

2.4 Merits of the computational methods based on the integral equations

Note that the popular today FDTD codes are not able to solve eigenvalue problems directly. Instead, they need a pulsed source placed inside a cavity, so that evaluation of the natural frequencies and Q-factors is done via spectral analysis of a transient signal [8,9]. On the other hand, the billiards theory neglects the field leakage to the host space and therefore fails to quantify the Q-factors. An attempt to improve this geometrical approach by using Fresnel coefficients has limited effect as it is based on the assumption of a locally flat boundary illuminated by a locally plane wave, and realistic microcavities are far from this situation. These difficulties are absent if one reduces the BVP to volume (VIE) or boundary (BIE) integral equations. VIEs have the advantage of being applicable even to cavities with non-uniform refractive indices. However, all 3-D and H-polarization 2-D VIEs are strongly singular that makes their application questionable because of the non-convergence of discrete schemes. This drawback was overcome in [10], where a regularisation procedure for 2-D VIEs was developed. In contrast, the E-polarised case leads to the Fredholm second kind 2-D VIEs and convergent algorithms. E.g., such a technique was developed in [11] to model a microdisk filter in a slab waveguide. This approach has clear advantages over such popular counterparts as the physically transparent, yet rough, coupled-mode approximations [12] and FDTD codes. The same VIEs, if extended into the complex-frequency domain, can be used for the accurate calculation of the Q-factors. Note that VIE combined with perturbation technique is a traditional tool for estimating the effect of surface roughness on the WG modes [13].

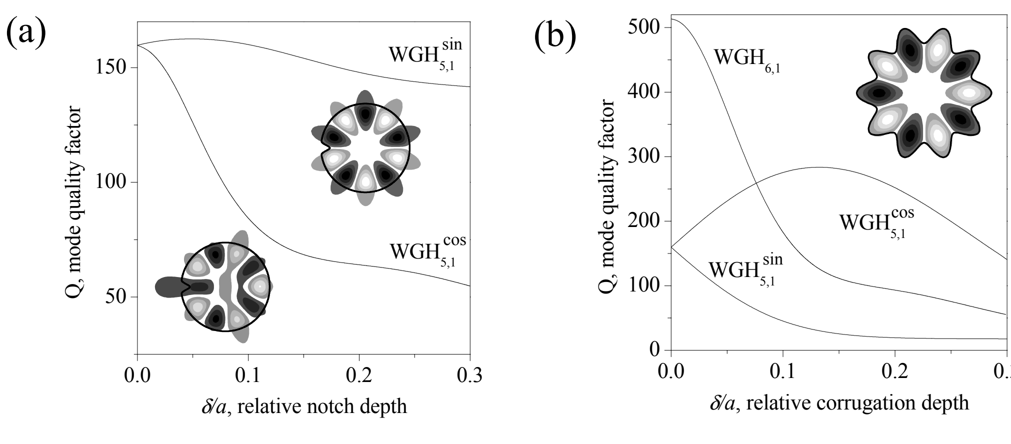

Figure 2.(a) Q-factors of the notch-matched and mismatched $(H_z)_{5,1}$ modes (see insets) in a notched disk [25] as a function of the notch depth normalised to the disk radius; (b) Q-factors of the deformation-matched (see inset) and mismatched $(H_z)_{m,1}$ modes in a "flower-shape" disk as a function of sinusoidal corrugation depth normalised to the disk radius; $\alpha = 3.374$, $\lambda = 1.55$ μm, disk thickness is $d = 200$ nm, effective index is $\alpha_{eff} = 2.63$.

BIE formulations are more economic than VIE ones due to lower dimensionality, although they work only if the refractive index is constant inside the cavity. BIEs can be easily cast into the form free of strong singularities. However, many forms of BIE possess an infinite number of discrete defect frequencies [14] – eigenvalues of the interior electromagnetic problem where the boundary *S* is assumed perfectly electrically conducting and filled with the outer-medium material (e.g., free space). In terms of the eigenvalue BVP it means that infinite number of false real-valued eigenfrequencies is present. Such a technique was developed in [15] and applied to the analysis of low-Q modes in passive non-circular cavities [15-17]. Another version of "defective" BIE was applied in [18] to study the enhancement of spontaneous emission in a more justified manner – only smaller than wavelength cavities were computed, i.e. the frequency remained lower than the first "defect" value. Analytical preconditioning may reduce the negative effect of the false eigenvalues although it does not remove them. Such a refined variant of "defective" 2-D BIE analysis has been successfully applied in [19, 20] to study the high-*Q* WG modes in circular and non-circular cavities in layered media.

Fortunately, there exists a perfectly reliable tool for the modal analysis of dielectric cavities. This is already mentioned Muller BIE (in fact, two coupled BIEs) because they are (i) free of defect frequencies and (ii) have smooth or integrable kernels. A Muller BIE can be discretised either with collocations [21] or with a Galerkin-type projection to global expansion functions [22]. Both ways possess a convergence thanks to the Fredholm second kind nature of Muller BIEs. According to [22], the size of the resultant matrix is determined by the electrical size of the cavity, normalised peak curvature of the boundary, and the desired accuracy (in digits) in almost equal manner. We emphasise this because, as a rule, the published works where BIEs are used ignore the last two parameters and blindly rely on the "rule-of-a-thumb" of taking 10 mesh points per wavelength. This powerful method has been already applied to the accurate 2-D analysis of optical modes in various non-circular passive dielectric cavities [22-25], including very high-Q-factor WG modes (see Fig. 2). Modal analysis of more realistic 3-D cavities with Muller BIEs remains a topic for future studies; it will accurately establish the domain of validity of the effective index based 2-D approximation.

3. LASING EIGENVALUE PROBLEMS: THRESHOLD AND THE ACTIVE REGION SHAPE

The main point, however, is that the lasing phenomenon is not addressed directly through the Q-factor – the specific value of the pump or gain that is needed to force a mode to become lasing is not included in the formulation. As a practical consequence, the Q-factor theory fails to explain why photopumping with a hollow beam reduces the threshold power for a microdisk [26] and why in the stadium-shape cavity the lasing occurs on the "bow-tie" modes [6], whose Q-factors are several orders lower than those of the WG-like modes. Trying to answer these questions, researchers resorted to complicated non-linear descriptions of the lasing [27,28].

On realising such a gap in the linear characterisation of lasers, one can modify the formulation of the electromagnetic problem by introducing macroscopic gain in the cavity material and extracting not only the frequencies but also the thresholds as eigenvalues. Here, material gain, say γ, is the *active* imaginary part of the complex refractive index ν: if the time dependence is assumed as e^{-ikct}, then $\nu = \alpha - i\gamma$, $\alpha, \gamma > 0$. Such a *lasing eigenvalue problem* (LEP) was suggested in [29]. The gain per unit length, the traditional quantity for Fabry-Perot cavities, is $g = k\gamma$, and, in principle, γ can be expressed via the medium microscopic parameters with the aid of the two-level model [28]. Note that, unlike the analysis of the scattering of light by active bodies (see [30]), the search of their LEP eigenvalues does not lead to non-physical results. To link the LEP with the more traditional Q-factor problem, one can keep in mind that each complex-valued eigenfrequency k_s is a continuous function of γ. In fact, in LEP we seek a specific value of $\gamma = \gamma_s$ that brings the function $\operatorname{Im} k_s(\gamma)$ to zero, and consider this as the threshold of lasing at which the radiation losses are balanced exactly with the macroscopic gain of active medium. The pair of real numbers, (k_s, γ_s), is therefore the signature of the *s*-th lasing mode. Note that, thanks to the real-valued *k*, modal fields do not diverge at infinity. Similarly to the complex eigenfrequencies, basic properties of the lasing eigenvalues can be established before their computation. It is found that (i) eigenvalues form a discrete set on the plane (k, γ); (ii) all $\gamma_s > 0$ and each has finite multiplicity; (iii) k_s and γ_s depend on geometry and α in piece-continuous or piece-analytic manner.

Application of the LEP approach to the circular resonator as a 2-D model of microdisk was presented in [30] and led to the accurate quantification of the thresholds of both WG and non-WG modes. Quasi-3-D features were further provided to the LEP analysis of a microdisk laser by an accurate account for the multiple-value character of the thin-disk effective index and for its dispersion. A non-uniform distribution of gain across the disk, due to either shaped pump beam or shaped electrodes cannot be accounted for in the passive cavity model but is easily accounted for in LEP. To this end, one has to introduce the gain only inside the active region and impose an additional set of transmission conditions on its boundary. In [31], such a 2-D LEP analysis was done for microdisks with active regions shaped as (i) a circle centred inside the disk and (ii) a ring adjacent to the disk rim; it has proven that placing the active region (e.g., an electrode of injection laser [32]) in the cavity centre boosts the thresholds of the WG modes by many orders of magnitude.

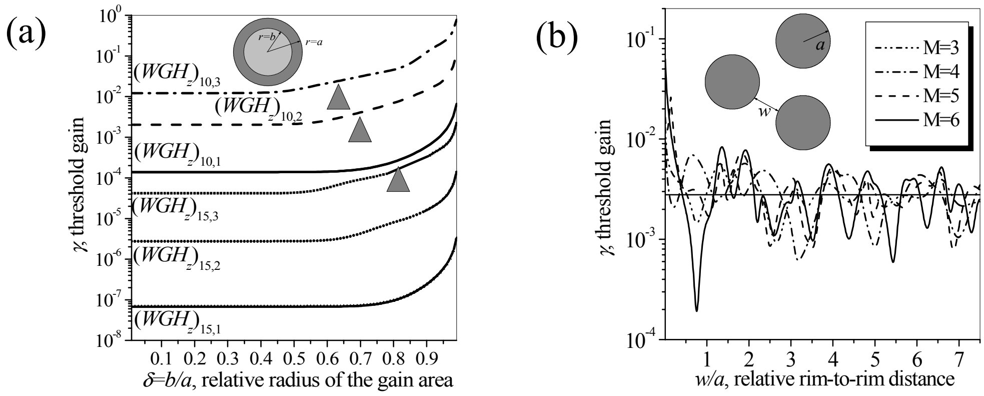

Figure 3 (a) Thresholds of the $(H_z)_{m1,0}$ modes in a GaAs disk with the ring-like active region as a function of its inner radius normalized to the disk radius [30]*; Triangles mark threshold values twice larger than for a uniformly active disk. (b) Thresholds versus the rim-to-rim air gap width normalized to the disk radius, for the lasing supermodes of the $(H_z)_{6,1}$ type of the maximally symmetric field class in the cyclic PMs* [34] *made of M microdisks. Straight line is the threshold of in the single cavity;* $\alpha = 3.374$ *,* $\lambda = 1.55$ *, and disk thickness* $d = 200$ *nm.*

In contrast, a ring-shape active region may be as narrow as 0.1*a* and still provide the same value of the material gain threshold as in the uniform-gain disk (Fig. 3*a*). Thus the intuitive idea of the importance of "spatial matching" between the active region and the modal field pattern is incorporated into the LEP automatically.

In [33], a twin-disk photonic-molecule (PM) laser has been studied, based on the reduction of the LEP to a Fredholm second kind matrix problem. Here, degenerate WG modes split into four orthogonal coupled modes (i.e., supermodes) of different symmetry classes. The most interesting result is that, for each of the supermodes, careful tuning of the distance between the disks may provide a threshold, which is lower than for a single cavity. Similar effect takes place for a two-disk PM with one active and another passive cavity and for PMs arranged as cyclic arrays of identical active microdisks [34]. For the latter PMs, a remarkable symmetry-assisted reduction of thresholds has been found for the supermodes built of the WG modes in individual cavities (see Fig. 3b), if the distance between the adjacent disks is properly tuned. This phenomenon is similar to the increase of Q-factors in a passive cavity reported in [35]. Thus, the idea of the authors of [36] was generally right although they had apparently selected a wrong distance between the WG-mode resonators in a cyclic PM laser and hence did not see the expected reduction of threshold.

Cold-cavity linear modelling of lasing thresholds of a microdisk equipped with single or several QDs is another example of a problem not tractable with a passive cavity model, however accessible through the LEP analysis. It is worthy of note that the finite spectral width of the photoluminescence of the active region can be taken into account in the LEP in the same manner as the dispersion of the effective index (see [31]). It is clear that, in such a formulation, only those lasing modes whose frequencies spectrally match the photoluminescence band will keep low thresholds.

4. CONCLUSIONS

We have reviewed the general framework for the analysis of electromagnetic fields in microcavities as eigensolutions to full Maxwellian BVPs. A reliable tool for their recovery must somehow tackle arbitrarily curved boundaries, use rigorous boundary conditions, and accurately account for the open host space; hence ray tracing and FDTD numerical codes are not good candidates. It must also be free of false eigenvalues. All these criteria are satisfied when using the technique based on the Muller BIEs. We have also discussed that to analyse the lasing in direct manner, though still within a linear formulation, one has to switch from a passive cavity to the cavity with gain in the active region, i.e., to study a LEP. In this case, analysis of Q-factors is replaced with analysis of the threshold values of material gain. In fact, the LEP can be called a "warm-cavity" model of laser as it takes into account, although in an averaged manner via the macroscopic concept of an "active" imaginary part of refractive index, the presence of carriers in semiconductor material.

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