Lasing eigenvalue problems: The electromagnetic modelling of microlasers

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Abstract

Comprehensive microcavity laser models should account for several physical mechanisms, e.g. carrier transport, heating and optical confinement, coupled by non-linear effects. Nevertheless, considerable useful information can still be obtained if all non-electromagnetic effects are neglected, often within an additional effective-index reduction to an equivalent 2D problem, and the optical modes viewed as solutions of Maxwell's equations. Integral equation (IE) formulations have many advantages over numerical techniques such as FDTD for the study of such microcavity laser problems. The most notable advantages of an IE approach are computational efficiency, the correct description of cavity boundaries without stair-step errors, and the direct solution of an eigenvalue problem rather than the spectral analysis of a transient signal. Boundary IE (BIE) formulations are more economic that volume IE (VIE) ones, because of their lower dimensionality, but they are only applicable to the constant cavity refractive index case. The Muller BIE, being free of 'defect' frequencies and having smooth or integrable kernels, provides a reliable tool for the modal analysis of microcavities. Whilst such an approach can readily identify complex-valued natural frequencies and Q-factors, the lasing condition is not addressed directly. We have thus suggested using a Muller BIE approach to solve a *lasing eigenvalue problem* (LEP), i.e. a linear eigenvalue solution in the form of two real-valued numbers (lasing wavelength and threshold information) when macroscopic gain is introduced into the cavity material within an active region. Such an approach yields clear insight into the lasing thresholds of individual cavities with uniform and non-uniform gain, cavities coupled as photonic molecules and cavities equipped with one or more quantum dots.

Keywords: microcavity lasers, integral equations, linear electromagnetic modelling, eigenvalue problem, linear threshold

A. Passive Cavities: Mathematical Study of 3-D Complex-Frequency Eigenvalue Problems

When studying time-harmonic electromagnetic fields in the presence of a dielectric microcavity, usually one implies that the cavity has finite volume V bounded with a smooth surface S, and that the host medium is free space. If, for simplicity, the cavity material is assumed uniform, i.e. it assumed that the refractive index is a constant, say α inside S, and 1 outside, then the natural, or source-free, electromagnetic field problem leads to the frequency eigenvalue problem [1]. It implies that one looks for the natural frequencies (for convenience, normalized by the light velocity c, i.e. the natural wavenumbers k) generating non-zero fields $\{\vec{E},\vec{H}\}e^{-ikct}$. These fields solve, off the cavity surface S, the set of *homogeneous time-harmonic Maxwell equations* with *transmission conditions*: that the tangential field components must be continuous across S. Further, the electromagnetic energy must be locally finite (i.e. integrable) to prevent source-like field singularities, and, eventually, one 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 [1], which provides for the outgoing spherical-wave behaviour

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and, in addition, eliminates non-transverse components of $\vec{E}$ and $\vec{H}$ at infinity. The set of conditions mentioned is "inherited" from the wave-scattering problems where they guarantee the uniqueness of the solution for all real values of *k*. Thus one arrives at an eigenvalue boundary-value problem (BVP).

Several important general properties of the eigenfrequencies can be found even before solving the formulated BVP. Thus, provided that the cavity material is passive, whatever is the open cavity geometry, real-valued eigenfrequencies cannot exist; while complex eigenvalues of *k* can be located only in the lower half-plane of the *k*-plane ($\mathrm{Im}\, k < 0$), for the selected time dependence. This corresponds to a damping with time due to radiation losses; for the same reason the field functions $\{\vec{E},\vec{H}\}$ diverge at infinity as $O(e^{-\mathrm{Im}\, kR} / R)$. In this sense, the eigenfrequencies of a passive open cavity are *generalized eigenvalues* generating *generalized eigenfunctions*. They come in pairs: if *k* is an eigenvalue, then so is –*k**; this is a consequence of the time invariance in harmonic problems.

Further, the eignevalue BVP can be equivalently reduced to a set of four coupled boundary integral equations (IEs) of the second kind with smooth or integrable kernels analytic on the complex *k*–plane (so-called Muller BIEs) [1, 2]. Therefore, the Fredholm theorems generalized for operators hold true [3, 4]. They tell us 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 each of them has finite multiplicity. Therefore, one can number them with an index, say *s*. Although this property seems to be almost evident from the physical point of view, it has important practical consequence in numerical modelling: there is no danger that an algorithm looking for k_s may hit a line or lacuna filled with eigenfrequencies. More important is that each k_s is a piecewise-continuous or piecewise-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 optical field function, and the entity of eigenfrequency and eigenfunction is considered as a *mode*. The quality factors of modes are defined as $Q_s = |\mathrm{Re}\, k_s / 2\,\mathrm{Im}\, k_s| > 0$. As mentioned, the eigenfrequencies may coincide, this is called *modal degeneracy*. If the degeneracy is caused by a 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, as well as the eigenfunction, a finite chain of *associated functions* appear; all together such functions are called *root functions*.

Unfortunately, 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, the set of generalized eigenmodes of an open cavity does not possess *completeness*, in a mathematical sense. Besides, orthogonality between the generalized 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 [5]. All this prevents one from using such modes as a discrete-mode functional basis in the scattering problems.

B. Thin Cavity Case: Generalized Boundary Conditions and Dimensionality Reduction to 2-D

If the cavity thickness is a fraction of both its diameter and the wavelength, one can simplify the BVP analysis by neglecting the electromagnetic field inside the cavity and treating it as a zero-thickness one. Mathematically, this approach is called *homogenisation* of the BVP. It leads to the modification of the boundary conditions across the cavity plane – the new form of such (generalized) conditions involves the jumps of tangential components of both $\vec{E}$ and $\vec{H}$ (i.e., equivalent magnetic and electric currents) with coefficients absorbing the actual thickness and material constants of the thin cavity. The BVP remains a 3-D one, however the complicated integration domain (cavity's surface *S*) in the associated boundary IE shrinks to a simpler 2-D domain in the plane of the cavity. Furthermore, in the case of thin cavity a total reduction of dimensionality of a microcavity BVP, from 3-D to 2-D, is tempting. At its core one finds the assumption that the field dependences on the normal-to-cavity-face (z) and in-plane (r,φ) coordinates are separable (see [6]). 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 the coefficient instead of the bulk refractive index as in the 3-D BVP. 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 [6]. 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, BVP can be also equivalently reduced to two coupled contour-type Muller's IEs with the same conclusions about the discreteness, finite multiplicity, and continuous dependence of eigenfrequencies on parameters. However, they are now located not on the complex *k*-plane but on the Riemann surface of the multi-valued function $\mathrm{Ln}k$. 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 $k=0$.

C. Merits of the Integral-Equation Based Computational Methods

Unfortunately, popular time-domain numerical codes, typified by the finite difference time domain (FDTD) method, are not able to solve eigenvalue problems directly – they always need a time-varying source placed inside a cavity; evaluation of the natural frequencies and Q-factors is done via spectral analysis of a transient signal [7,8]. Therefore the results obtained can depend on the location of the source and observation points and other not physically relevant factors. On the other hand, billiards theory [9] 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 a 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, a fact which 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. For example, 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 time-domain numerical codes. The same VIEs, if extended into the complex-frequency domain, can be used for the accurate calculation of the Q-factors.

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 a form free of strong singularities. However, many forms of BIE possess an infinite number of discrete defect frequencies [13] – 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 an infinite number of false real-valued eigenfrequencies is present. Such a technique was developed in [14] and applied to the analysis of low-Q modes in passive non-circular cavities [14, 15]. Another version of "defective" BIE was applied in [16] 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. Analytic pre-conditioning 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 [17, 18] to study the high-Q whispering-gallery (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 the Muller BIE (in fact, two coupled BIEs) already mentioned which are (i) free of defect frequencies and (ii) have smooth or integrable kernels. A Muller BIE can be discretised either with collocations [19] or with a Galerkin-type projection to global expansion functions [20]. Both ways possess a guaranteed convergence thanks to the Fredholm second kind nature of Muller BIEs. According to [20], 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 [20-23], including very high-Q-factor WG modes. The 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.

D. Lasing: Active Region and Threshold Value of Material Gain

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 photo-pumping with a hollow beam reduces the threshold power for a microdisk [24] and why in the stadium-shape cavity the lasing occurs on the "bow-tie" modes [9] whose Q-factors are several orders lower than those of the WG-like modes. Trying to answer these questions, researchers have resorted to complicated non-linear descriptions of the lasing [25, 26].

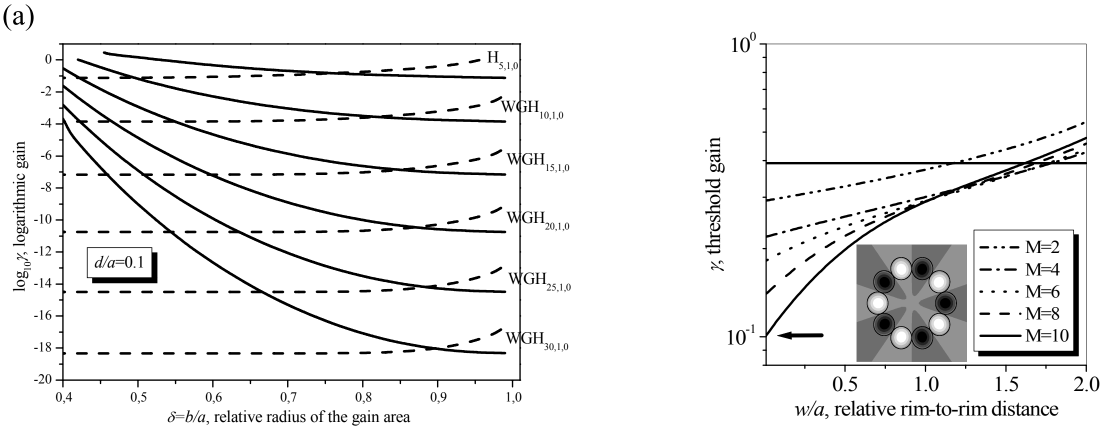
On realising such a gap in the linear characterisation of lasers, we have modified the formulation of the electromagnetic problem by introducing macroscopic gain in the cavity material and extracting not only the frequencies but also the thresholds as eigenvalues. Here, material gain, say γ, is the *active* 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 [27]. 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 [26]. Note that, unlike the analysis of the scattering of light by active bodies (see [28]), 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, the basic properties of the lasing eigenvalues can be established before their computation: (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 bulk refractive index α in a piecewise-continuous or piecewise-analytic manner.

Application of the LEP approach to the circular resonator as a 2-D model of microdisk was presented in [27] 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 [6]. 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 [6], 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 was proven that placing the active region (e.g., an electrode of injection laser [29]) in the cavity centre boosts the thresholds of the WG modes by many orders of magnitude.

In contrast, a ring-shape active region may be as narrow as $0.1a$ and still provide the same value of the material gain threshold as in the uniform-gain disk (see Fig. 1-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. Note that the crossing of the solid and dashed curves in Fig. 1-a takes place at the level of the doubling of the threshold, for each mode, relatively to the uniformly active disk threshold. This is because here the active region, shaped as either an inner circle or a ring adjacent to the cavity rim, overlaps with exactly a half of the modal field power.

(a)



(b)

Figure 1.(a) Threshold values of the whispering-gallery $(H_z)_{m,1}$ modes in a thin-disk cavity [6] with radially non-uniform gain as a function of the gain-to-rim radii ratio; (b) Thresholds versus the rim-to-rim airgap width normalized to the disk radius, for the lasing supermodes of the π-$(H_z)_{0,1}$ type in the cyclic PMs [32] made of *M* active microdisks; straight line is the threshold of in the single cavity. Bulk refractive index $\alpha = 3.374$, wavelength $\lambda = 1.55$, disk thickness $d = 200$ nm (a) and $d = 100$ nm (b).

In [30], 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 [31]. 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, if the distance between the adjacent disks is properly tuned. Even more interesting is the effect of lowering the thresholds of lasing in a cyclic PM for the π-type supermodes built on the lowest possible elementary modes, such as monopole mode $(H_z)_{01}$ and dipole modes $(H_z)_{01}$, which never show a WG-type behaviour [32]. This happens provided that the elementary side-cavity disks are brought together, there is an even number of them, and this number is large (see Fig. 1-b).

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 [6]). It is clear that, in such a formulation, only those lasing modes whose frequencies spectrally match the photoluminescence band will keep low thresholds.

Conclusions

Linear analysis of the natural (i.e., source-free) electromagnetic fields in dielectric microcavities leads to the study of eigensolutions to Maxwellian BVPs. A reliable tool for their solution must somehow tackle arbitrarily curved boundaries, use rigorous boundary conditions, and accurately account for the open host space. All these criteria are fully satisfied when using the technique based on the Muller BIEs. To extend this analysis to the lasing in semiconductor cavities, though still remain 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, the search for the modal Q-factors should be replaced with search for the threshold values of material gain, for each of the optical modes. The LEP formulation takes into account, in an averaged manner via the macroscopic concept of an "active" imaginary part of refractive index, the presence of carriers in semiconductor material. Thus, it can be called a "warm-cavity" model of laser – an intermediate one between “cold” model, or passive cavity and “hot” model, or nonlinear model with the account of microscopic properties of the carriers.

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