COMPUTER RESEARCH AND MODELING 2019 VOL. 11 NO. 6 P. 1083–1090

DOI: 10.20537/2076-7633-2019-11-6-1083-1090

THE 3RD BRICS MATHEMATICS CONFERENCE

UDC: 517.958:621.373.8

Mathematical and numerical modeling of a drop-shaped microcavity laser

A. O. Spiridonov^{1,a}, E. M. Karchevskii^{2,b}

¹Laboratory of Computational Technologies and Computer Modeling, Kazan Federal University, 18 Kremlevskaya st., Kazan, 420008, Russia ²Department of Applied Mathematics, Kazan Federal University,

18 Kremlevskaya st., Kazan, 420008, Russia

E-mail: ^a aospiridonov@gmail.com, ^b ekarchev70@gmail.com

Received 23.05.2019. Accepted for publication 14.11.2019.

This paper studies electromagnetic fields, frequencies of lasing, and emission thresholds of a drop-shaped microcavity laser. From the mathematical point of view, the original problem is a nonstandard two-parametric eigenvalue problem for the Helmholtz equation on the whole plane. The desired positive parameters are the lasing frequency and the threshold gain, the corresponding eigenfunctions are the amplitudes of the lasing modes. This problem is usually referred to as the lasing eigenvalue problem. In this study, spectral characteristics are calculated numerically, by solving the lasing eigenvalue problem on the basis of the set of Muller boundary integral equations, which is approximated by the Nyström method. The Muller equations have weakly singular kernels, hence the corresponding operator is Fredholm with zero index. The Nyström method is a special modification of the polynomial quadrature method for boundary integral equations with weakly singular kernels. This algorithm is accurate for functions that are well approximated by trigonometric polynomials, for example, for eigenmodes of resonators with smooth boundaries. This approach leads to a characteristic equation for mode frequencies and lasing thresholds. It is a nonlinear algebraic eigenvalue problem, which is solved numerically by the residual inverse iteration method. In this paper, this technique is extended to the numerical modeling of microcavity lasers having a more complicated form. In contrast to the microcavity lasers with smooth contours, which were previously investigated by the Nyström method, the drop has a corner. We propose a special modification of the Nyström method for contours with corners, which takes also the symmetry of the resonator into account. The results of numerical experiments presented in the paper demonstrate the practical effectiveness of the proposed algorithm.

Keywords: microcavity laser, lasing eigenvalue problem, Muller boundary integral equation, Nyström method

Citation: *Computer Research and Modeling*, 2019, vol. 11, no. 6, pp. 1083–1090. This work was supported, in part, by RFBR via the research project No. 18-31-00026.

© 2019 Alexander O. Spiridonov, Evgenii M. Karchevskii This work is licensed under the Creative Commons Attribution-NoDerivs 3.0 Unported License. To view a copy of this license, visit http://creativecommons.org/licenses/by-nd/3.0/ or send a letter to Creative Commons, PO Box 1866, Mountain View, CA 94042, USA.

Ки&М

1. Introduction

Microcavity lasers have many promising applications in optoelectronics and photonics [Lebental et al., 2009]. If optical microcavities are thin and flat, then they can be investigated using twodimensional models [Smotrova et al., 2005]. Spectral characteristics of disk-like microcavity lasers were numerically analyzed by the Lasing Eigenvalue Problem (LEP) starting with the pioneering works [Smotrova et al., 2005], [Smotrova, Nosich, 2004]. Lately, LEP has been effectively used also for computer simulations of plasmonic nanolasers [Shapoval et al., 2017], [Natarov et al., 2019]. LEP has two real-valued eigenvalues: the frequency of lasing and the mode threshold gain. This statement is attractive for the optoelectronics and photonics community since, unlike the classical Complex-Frequency Eigenvalue Problem (developed for passive cavities), it describes the gain material of the cavity [Smotrova et al., 2011].

To solve LEP numerically, nonlinear spectral problems for systems of boundary integral equations were proposed in [Karchevskii, Nosich, 2014], [Nosich, 2016]. The kernels of the systems are weakly singular, therefore the corresponding operators are Fredholm with zero index. As a result, many efficient and theoretically justified numerical methods can be applied. One is the most attractive numerical techniques is the Nyström method presented in [Smotrova et al., 2013] and used recently in [Spiridonov et al., 2015]– [Spiridonov et al., 2017].

Developing the ideas of the articles cited in the previous paragraph, we have proposed a convenient (for numerical analysis operator) formulation of LEP [Spiridonov et al., 2018] and have constructed a modification of the Nyström method taking the symmetry of the problem [Spiridonov, Karchevskii, 2016] into account. What is important is that all the authors proceeded from the assumption that the boundary of the cavity was smooth. The current paper proposes an approach to mathematical and numerical modeling of a drop-shaped active microcavity. In the case of a drop shape, there is an angle, so we modify the Nyström method by conversion from the previously used uniform grid to a nonuniform grid with a concentration of points near the corner. Using this approach, we numerically analyze the spectra, thresholds, and the modal fields.

2. Statement of the problem

Consider a two-dimensional fully active drop-shaped microcavity laser (see Fig. 1). We assume that the refractive index in the active domain Ω_i is complex-valued, $\nu_i = \alpha_i - i\gamma$, where $\gamma > 0$ is the unknown threshold gain, and $\alpha_i > 0$ is known. In the environment Ω_o the refractive index is realvalued and positive, $\nu_o = \alpha_o > 0$. Denote by Γ the boundary of the domain Ω_i except for the corner point. Assume that the curve Γ defined in this way is twice continuously differentiable. Denote by nthe outer normal unit vector of the curve Γ . As usual, by k we denote the wave number assuming that the electromagnetic field harmonically depends on time. We are looking for sufficiently smooth (having



Figure 1. Geometry of a drop-shaped microcavity laser

finite energy in the neighborhood of the corner) nonzero functions u and corresponding eigenvalues of k > 0 and $\gamma > 0$ such that all the following equations are satisfied:

$$\Delta u(x) + k_j^2 u(x) = 0, \quad x \in \Omega_j, \quad j = i, o, \tag{1}$$

$$u^{-} = u^{+}, \quad \eta_{i} \frac{\partial u}{\partial n} = \eta_{e} \frac{\partial u^{+}}{\partial n}, \quad x \in \Gamma,$$
 (2)

$$u(r,\varphi) = \sqrt{\frac{2}{i\pi k_o r}} e^{ik_o r} \Phi(\varphi), \quad r \to \infty.$$
(3)

Here $k_{i/o} = k\nu_{i/o}$, $u = H_z$, $\eta_{i/o} = \nu_{i/o}^{-2}$ for the H-polarized electromagnetic field, and $u = E_z$, $\eta_i = \eta_o = 1$ for the E-polarized field. In the Sommerfeld radiation condition (3), by $\Phi(\varphi)$ we denote the far-field angular emission pattern. As usual, we denote the polar coordinates of the point x by (r, φ) , and the limits of u from inside and outside of Γ , by u^- and u^+ , respectively.

We use the well-known integral representations

$$u(x) = -\int_{\Gamma} \left(u^{-}(y) \frac{\partial G_{i}(x,y)}{\partial n(y)} - G_{i}(x,y) \frac{\partial u^{-}(y)}{\partial n(y)} \right) dl(y), \quad x \in \Omega_{i},$$
(4)

$$u(x) = \int_{\Gamma} \left(u^+(y) \frac{\partial G_o(x,y)}{\partial n(y)} - G_o(x,y) \frac{\partial u^+(y)}{\partial n(y)} \right) dl(y), \quad x \in \Omega_o,$$
(5)

where $G_{i/o}(x,y) = \frac{i}{4}H_0^{(1)}(k_{i/o}|x-y|)$, and reduce the original problem (1)–(3) to the following nonlinear eigenvalue problem for the system of boundary integral equations:

$$u(x) - \int_{\Gamma} K_{1,1}(x,y)u(y)dl(y) - \int_{\Gamma} K_{1,2}(x,y)v(y)dl(y) = 0,$$
(6)

$$v(x) - \int_{\Gamma} K_{2,1}(x,y)u(y)dl(y) - \int_{\Gamma} K_{2,2}(x,y)v(y)dl(y) = 0,$$
(7)
$$n_0 + n_i \,\partial u^- \qquad n_0 + n_i \,\partial u^+$$

$$u = u^{-} = u^{+}, \quad v = \frac{\eta \delta + \eta_{1}}{2\eta_{o}} \frac{\delta w}{\partial n} = \frac{\eta \delta + \eta_{1}}{2\eta_{i}} \frac{\delta w}{\partial n},$$

$$K_{1,1}(x, y) = \frac{\partial G_{o}(x, y)}{\partial n(y)} - \frac{\partial G_{i}(x, y)}{\partial n(y)}, \quad K_{1,2}(x, y) = \frac{2(\eta_{o}G_{i}(x, y) - \eta_{i}G_{o}(x, y))}{\eta_{o} + \eta_{i}},$$

$$K_{2,1}(k, \gamma; x, y) = \frac{\partial^{2}G_{o}(k; x, y)}{\partial n(x)\partial n(y)} - \frac{\partial^{2}G_{i}(k, \gamma; x, y)}{\partial n(x)\partial n(y)},$$

$$K_{2,2}(k, \gamma; x, y) = \frac{2}{\eta_{o} + \eta_{i}} \left(\frac{\eta_{o}\partial G_{i}(x, y)}{\partial n(x)} - \frac{\eta_{i}\partial G_{o}(x, y)}{\partial n(x)}\right).$$
(8)

3. Nyström method

In this section, for numerical solution of the problem (6)–(7), we construct the Nyström method. In the computations, we use the following parametrization of the boundary of the drop-shaped microcavity [Colton, Kress, 2013]:

$$r(t) = \left(a\sin\left(\frac{t}{2}\right) - \frac{a}{2}, \ b\sin(t)\right), \quad t \in [0, 2\pi].$$

2019, Vol. 11, No. 6, P. 1083–1090

Clearly, this curve has the corner at t = 0 (see Fig. 1). The kernels $K_{i,j}$ defined in the previous section are weakly singular and we can write them in the form

$$K_{i,j}(t,\tau) = Q_{i,j}(t,\tau) \ln\left(4\sin^2\frac{t-\tau}{2}\right) + P_{i,j}(t,\tau), \quad i,j = 1,2,$$
(9)

where functions $Q_{i,j}(t,\tau)$ and $P_{i,j}(t,\tau)$ are continuous on $[0,2\pi] \times [0,2\pi]$.

Following [Colton, Kress, 2013], we introduce the strictly monotonically increasing and infinitely differentiable function $\omega: [0, 2\pi] \rightarrow [0, 2\pi]$ so that

$$\omega(s) = 2\pi \frac{[\upsilon(s)]^p}{[\upsilon(s)]^p + [\upsilon(2\pi - s)]^p}$$

where $s \in [0, 2\pi]$, $p \ge 2$ and

$$v(s) = \left(\frac{1}{p} - \frac{1}{2}\right) \left(\frac{\pi - s}{\pi}\right)^3 - \frac{1}{p}\frac{\pi - s}{\pi} + \frac{1}{2}.$$

Denote by \mathbb{N} the set all positive integers, and take $n \in \mathbb{N}$. By $\widetilde{\Xi}_n = \{s_j\}_{j=0}^{2n-1}$ we denote the uniform grid on the interval $[0, 2\pi]$. The mesh size of this grid is $h = \pi/n$, and $s_j = j\pi$, $j = 0, \ldots, 2n - 1$. Then the grid $\Xi_n = \{t_j\}_{j=0}^{2n-1}$, where $t_j = \omega(s_j)$, is nonuniform.

Using the representation $t = \omega(s), \tau = \omega(\sigma)$, we obtain

$$\int_{0}^{2\pi} K_{i,j}(t,\tau)\psi(\tau)d\tau = \int_{0}^{2\pi} K_{i,j}(\omega(s),\omega(\sigma))\psi(\omega(\sigma))\omega'(\sigma)d\sigma$$

and write

$$K_{i,j}(t,\tau) = K_{i,j}(\omega(s),\omega(\sigma)) = \widetilde{Q}_{i,j}(s,\sigma)\ln\left(4\sin^2\frac{s-\sigma}{2}\right) + \widetilde{P}_{i,j}(s,\sigma), \quad i,j = 1,2.$$

The following decompositions are related to (9):

$$\widetilde{Q}_{i,j}(s,\sigma) = Q_{i,j}(\omega(s),\omega(\sigma)),$$

and

$$\widetilde{P}_{i,j}(s,\sigma) = \begin{cases} K_{i,j}(\omega(s),\omega(\sigma)) - \widetilde{Q}_{i,j}(s,\sigma)\ln\left(4\sin^2\frac{s-\sigma}{2}\right), & s \neq \sigma, \\ P_{i,j}(\omega(s),\omega(s)) - 2\ln\omega'(s)Q_{i,j}(\omega(s),\omega(s)), & s = \sigma. \end{cases}$$

Using the representations $\tau_j = \omega(\sigma_j)$, $a_j = \omega'(\sigma_j)$, $\tilde{r}(\sigma) = r(\omega(\sigma))$, we write the approximate solution of the problem (6)–(7) as follows:

$$u^{(n)}(s) = \sum_{j=1}^{2n-1} a_j \left(R_j^{(n)}(s) \widetilde{Q}_{1,1}(s,\sigma_j) + \frac{\pi}{n} \widetilde{P}_{1,1}(s,\sigma_j) \right) |\widetilde{r'}(\sigma_j)| u_j + \sum_{j=1}^{2n-1} a_j \left(R_j^{(n)}(t) \widetilde{Q}_{1,2}(s,\sigma_j) + \frac{\pi}{n} \widetilde{P}_{1,2}(s,\sigma_j) \right) |\widetilde{r'}(\sigma_j)| v_j, \quad (10)$$
$$v^{(n)}(s) = \sum_{j=1}^{2n-1} a_j \left(R_j^{(n)}(s) \widetilde{Q}_{2,1}(s,\sigma_j) + \frac{\pi}{n} \widetilde{P}_{2,1}(s,\sigma_j) \right) |\widetilde{r'}(\sigma_j)| u_j + \sum_{j=1}^{2n-1} a_j \left(R_j^{(n)}(s) \widetilde{Q}_{2,2}(s,\sigma_j) + \frac{\pi}{n} \widetilde{P}_{2,2}(t,\sigma_j) \right) |\widetilde{r'}(\sigma_j)| v_j, \quad (11)$$

COMPUTER RESEARCH AND MODELING

where
$$|\tilde{r'}(\sigma)| = \sqrt{(r'_1(\omega(\sigma))^2 + (r'_2(\omega(\sigma)))^2)}, s, \sigma \in [0, 2\pi], u_i = u(\omega(s_i)), v_i = v(\omega(s_i)),$$

$$R_j^{(n)}(s) = -\frac{2\pi}{n} \sum_{m=1}^{n-1} \frac{1}{m} \cos m(s - s_j) - \frac{\pi}{n^2} \cos n(s - s_j), \quad i, j = 1, \dots, 2n - 1.$$

It is important to note that $a_0 = 0$. The unknown values u_j and v_j , j = 0, ..., 2n - 1, satisfy the following system of linear algebraic equations:

$$u_{i} - \sum_{j=1}^{2n-1} a_{j} \left(R_{|i-j|}^{(n)} \widetilde{Q}_{1,1}(s_{i}, s_{j}) + \frac{\pi}{n} \widetilde{P}_{1,1}(s_{i}, s_{j}) \right) |\widetilde{r'}(s_{j})| u_{j} - \sum_{j=1}^{2n-1} a_{j} \left(R_{|i-j|}^{(n)} \widetilde{Q}_{1,2}(s_{i}, s_{j}) + \frac{\pi}{n} \widetilde{P}_{1,2}(s_{i}, s_{j}) \right) |\widetilde{r'}(s_{j})| v_{j} = 0, \quad (12)$$

$$v_{i} - \sum_{j=1}^{2n-1} \left(R_{|i-j|}^{(n)} \widetilde{Q}_{2,1}(s_{i}, s_{j}) + \frac{\pi}{n} \widetilde{P}_{2,1}(s_{i}, s_{j}) \right) |\widetilde{r'}(s_{j})| u_{j} - \sum_{j=1}^{2n-1} a_{j} \left(R_{|i-j|}^{(n)} \widetilde{Q}_{2,2}(s_{i}, s_{j}) + \frac{\pi}{n} \widetilde{P}_{2,2}(s_{i}, s_{j}) \right) |\widetilde{r'}(s_{j})| v_{j} = 0, \quad (13)$$

where i = 0, ..., 2n - 1 and

$$R_j^{(n)} = R_j^{(n)}(0) = -\frac{2\pi}{n} \sum_{m=1}^{n-1} \frac{1}{m} \cos \frac{mj\pi}{n} - \frac{(-1)^j\pi}{n^2}, \quad j = 0, \dots, 2n-1.$$

Note that the matrix entries in (12) and (13) nonlinearly depend on the desired parameters k > 0 and $\gamma > 0$. Thus, we get the nonlinear algebraic spectral problem, which we solve numerically.

4. Numerical results

In our computations we use a = 2, b = 1, p = 8 and find H-polarized modes of the drop-shaped microcavity laser with the refractive index $\alpha = 2.63$, which is the effective value of the refractive index for a 200-nm GaAs skin in the infrared spectrum. The curve Γ is symmetric with respect to the x_1 axis. Following [Spiridonov et al., 2017], we calculate solutions having the same symmetry or antisymmetry. Figures 2 and 3 present semilog color maps of the inverse condition number of the matrix A of the system (6)–(7) on the plane (κ, γ) for x_1 -even and x_1 -odd modes of the drop-shaped microcavity laser, respectively. Using the local minima indicated in Figs. 2, 3 as initial approximations for the method of inverse iterations, we obtain solutions presented in Fig. 4.

Figure 5 shows the near and far fields for some of the modes appearing in Fig. 4. Analyzing the patterns for the near fields, we conclude that the thresholds are lower for those modes in which the field is aligned along the rounded part of the boundary.

5. Conclusion

In this paper we have proposed and studied a new modification of the Nyström method specially tailored for domains with corners. We applied this method for numerical calculations of emission characteristics of drop-shaped microcavity lasers. In our forthcoming work we are going to investigate the convergence of this method theoretically.



Figure 2. The inverse condition number of the matrix A as a function of the parameters $\kappa = ka$ and γ for x_1 -even modes of the drop-shaped microcavity laser



Figure 3. The inverse condition number of the matrix A as a function of the parameters $\kappa = ka$ and γ for x_1 -odd modes of the drop-shaped microcavity laser



Figure 4. Normalized emission frequencies and the corresponding threshold gains for the modes of the dropshaped microcavity laser. Red pluses denote even modes, blue crosses denote odd modes



Figure 5. Some modes of a drop-shaped microcavity laser. Here, ka is the normalized frequency of lasing, γ is the threshold gain, D is the directivity of the mode

References

- Colton D., Kress R. Inverse Acoustic and Electromagnetic Scattering Theory. New York: Springer, 2013.
- *Karchevskii E., Nosich A.* Methods of analytical regularization in the spectral theory of open waveguides // Proc. Int. Conf. Math. Methods in EM Theory (MMET*2014). 2014. P. 39–45.
- *Lebental M., Bogomolny E., Zyss J.* Organic micro-lasers: a new avenue onto wave chaos physics // in A. B. Matsko (Ed.) Practical Applications of Microresonators in Optics and Photonics, CRC Press, Roca Baton. 2009. P. 317–353.
- Natarov D. M., Benson T. M., Nosich A. I. Electromagnetic analysis of the lasing thresholds of hybrid plasmon modes of a silver tube nanolaser with active core and active shell // Beilstein J. Nanotechnology. - 2019. - Vol. 10. - P. 294-304.
- *Nosich A. I.* Method of analytical regularization in computational photonics // Radio Science. 2016. Vol. 51, No. 8. P. 1421–1430.
- Shapoval O. V., Kobayashi K., Nosich A. I. Electromagnetic engineering of a single-mode nanolaser on a metal plasmonic strip placed into a circular quantum wire // IEEE J. Sel. Topics Quant. Electron. – 2017. – Vol. 23, No. 6. – Art. no. 1501609.
- Smotrova E. I., Nosich A. I., Benson T. M., Sewell P. Cold-cavity thresholds of microdisks with uniform and non-uniform gain: quasi-3D modeling with accurate 2D analysis // IEEE J. Sel. Topics Quant. Electron. – 2005. – Vol. 11. – P. 1135–1142.
- Smotrova E. I., Byelobrov V. O., Benson T. M., et al. Optical theorem helps understand thresholds of lasing in microcavities with active regions // IEEE J. Quant. Electron. – 2011. – Vol. 47, No. 1. – P. 20–30.
- Smotrova E. I., Tsvirkun V., Gozhyk I., et al. Spectra, thresholds, and modal fields of a kite-shaped microcavity laser // J. Opt. Soc. Am. B. 2013. Vol. 30, No. 6. P. 1732–1742.
- Smotrova E. I., Nosich A. I. Mathematical study of the two-dimensional lasing problem for the whispering-gallery modes in a circular dielectric microcavity // Opt. Quant. Electron. – 2004. – Vol. 36. – P. 213–221.

- Spiridonov A. O., Karchevskii E. M. Field patterns of whispering-gallery and bow-tie modes of elliptic microcavity laser with a circular active region // Proc. Int. Conf. Transp. Opt. Networks (ICTON-2016). – 2016. – Art. No. 7550639.
- Spiridonov A. O., Karchevskii E. M. Mathematical and numerical analysis of the spectral characteristics of dielectric microcavities with active regions // Proc. Int. Conf. Days on Diffraction (DD-2016). – 2016. – P. 390–395.
- Spiridonov A. O., Karchevskii E. M. Benson T. M., Nosich A. I. Why elliptic microcavity lasers emit light on bow-tie-like modes instead of whispering-gallery-like modes // Opt. Comm. – 2019. – Vol. 439. – P. 112–117.
- Spiridonov A. O., Karchevskii E. M., Nosich A. I. Spectra, thresholds, and modal fields of a circular microcavity laser transforming into a square // Proc. Int. Conf. Transp. Opt. Networks (ICTON-2015). – 2015. – Art. No. 7193654.
- Spiridonov A. O., Karchevskii E. M., Nosich A. I. Symmetry accounting in the integral-equation analysis of the lasing eigenvalue problems for two-dimensional optical microcavities // J. Opt. Soc. Am. B. – 2017. – Vol. 34. – P. 1435–1443.
- Spiridonov A. O., Karchevskii E. M., Nosich A. I. Rigorous formulation of the lasing eigenvalue problem as a spectral problem for a Fredholm operator function // Lobachevskii J. Math. – 2018. – Vol. 39. – P. 1148–1157.
- Zolotukhina A. S., Spiridonov A. O., Karchevskii E. M., Nosich A. I. Lasing modes of a microdisk with a ring gain area and of an active microring // Opt. Quant. Electron. 2015. Vol. 47, No. 12. P. 3883–3891.
- Zolotukhina A. S., Spiridonov A. O., Karchevskii E. M., Nosich A. I. Electromagnetic analysis of optimal pumping of a microdisk laser with a ring electrode // Appl. Phys. B. 2017. Vol. 123. Art. No. 32.