Benchmarking five numerical simulation techniques for computing resonance wavelengths and quality factors in photonic crystal membrane line defect cavities

We present numerical studies of two photonic crystal membrane microcavities, a short line-defect cavity with relatively low quality (Q) factor and a longer cavity with high Q. We use five state-of-the-art numerical simulation techniques to compute the cavity Q factor and the resonance wavelength ($\lambda$) for the fundamental cavity mode in both structures. For each method, the relevant computational parameters are systematically varied to estimate the computational uncertainty. We show that some methods are more suitable than others for treating these challenging geometries.
Benchmarking state-of-the-art numerical simulation techniques for analyzing large photonic crystal membrane line defect cavities

In this work, we perform numerical studies of two photonic crystal membrane microcavities, a short line-defect L5 cavity with relatively low quality (Q) factor and a longer L9 cavity with high Q. We compute the cavity Q factor and the resonance wavelength $\lambda$ of the fundamental M1 mode in the two structures using five state-of-the-art computational methods. We study the convergence and the associated numerical uncertainty of Q and $\lambda$ with respect to the relevant computational parameters for each method. Convergence is not obtained for all the methods, indicating that some are more suitable than others for analyzing photonic crystal line defect cavities.

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Benchmarking state-of-the-art optical simulation methods for analyzing large nanophotonic structures

Five computational methods are benchmarked by computing quality factors and resonance wavelengths in photonic crystal membrane L5 and L9 line defect cavities. Careful convergence studies reveal that some methods are more suitable than others for analyzing these cavities.

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Organisations: Department of Photonics Engineering, Nanophotonics Theory and Signal Processing, Nanophotonic Devices, Department of Electrical Engineering, Electromagnetic Systems, Department of Mechanical Engineering, Solid Mechanics, Plasmonics and Metamaterials, St. Petersburg National Research University of Information Technologies, Mechanics and Optics (ITMO), Zuse Institute Berlin
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High quality factor GaAs microcavity with buried bullseye defects

The development of high quality factor solid-state microcavities with low mode volumes has paved the way towards on-chip cavity quantum electrodynamics experiments and the development of high-performance nanophotonic devices. Here, we report on the implementation of a new kind of solid-state vertical microcavity, which allows for confinement of the electromagnetic field in the lateral direction without deep etching. The confinement originates from a local elongation of the cavity layer imprinted in a shallow etch and epitaxial overgrowth technique. We show that it is possible to improve the quality factor of such microcavities by a specific in-plane bullseye geometry consisting of a set of concentric rings with subwavelength dimensions. This design results in a smooth effective lateral photonic potential and therefore in a reduction of lateral scattering losses, which makes it highly appealing for experiments in the framework of exciton-polariton physics demanding tight spatial confinement.

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Organisations: Department of Photonics Engineering, Nanophotonics Theory and Signal Processing, University of Würzburg
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Which Computational Methods Are Good for Analyzing Large Photonic Crystal Membrane Cavities?
By introducing defects into an otherwise periodic photonic crystal lattice, high quality (Q) factor cavities may be formed. However, the size and the lack of simplifying symmetries in the photonic crystal membrane make these types of cavities exceptionally hard to analyze using numerical simulation methods. In this work, we consider two different line defect cavities and we compute their Q factors using state-of-the-art optical simulation tools. We show that certain simulation methods perform much better than others in the analysis of these challenging structures.

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Organisations: Department of Photonics Engineering, Plasmonics and Metamaterials, Nanophotonics Theory and Signal Processing, Nanophotonic Devices, Department of Electrical Engineering, Electromagnetic Systems, Department of Mechanical Engineering, Solid Mechanics, Zuse Institute Berlin, St. Petersburg National Research University of Information Technologies, Mechanics and Optics (ITMO)
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**Interference-exact radiative transfer equation**

The Purcell effect, i.e., the modification of the spontaneous emission rate by optical interference, profoundly affects the light-matter coupling in optical resonators. Fully describing the optical absorption, emission, and interference of light hence conventionally requires combining the full Maxwell’s equations with stochastic or quantum optical source terms accounting for the quantum nature of light. We show that both the nonlocal wave and local particle features associated with interference and emission of propagating fields in stratified geometries can be fully captured by local damping and scattering coefficients derived from the recently introduced quantized fluctuational electrodynamics (QFED) framework. In addition to describing the nonlocal optical interference processes as local directionally resolved effects, this allows reformulating the well known and widely used radiative transfer equation (RTE) as a physically transparent interference-exact model that extends the useful range of computationally efficient and quantum optically accurate interference-aware optical models from simple structures to full optical devices.
Benchmarking five computational methods for analyzing large photonic crystal membrane cavities

We benchmark five state-of-the-art computational methods by computing quality factors and resonance wavelengths in photonic crystal membrane L5 and L9 line defect cavities. The convergence of the methods with respect to resolution, degrees of freedom and number of modes is investigated. Convergence is not obtained for some of the methods, indicating that some are more suitable than others for analyzing line defect cavities.

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Comparison of Five Computational Methods for Computing Q Factors in Photonic Crystal Membrane Cavities

Five state-of-the-art computational methods are benchmarked by computing quality factors and resonance wavelengths in photonic crystal membrane L5 and L9 line defect cavities. The convergence of the methods with respect to resolution, degrees of freedom and number of modes is investigated. Special attention is paid to the influence of the size of the computational domain. Convergence is not obtained for some of the methods, indicating that some are more suitable than others for analysing line defect cavities.

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Comparison of Five Numerical Methods for Computing Quality Factors and Resonance Wavelengths in Photonic Crystal Membrane Cavities

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Enhanced Photon Extraction from a Nanowire Quantum Dot Using a Bottom-Up Photonic Shell
Semiconductor nanowires offer the possibility to grow high-quality quantum-dot heterostructures, and, in particular, CdSe quantum dots inserted in ZnSe nanowires have demonstrated the ability to emit single photons up to room temperature. In this paper, we demonstrate a bottom-up approach to fabricate a photonic fiberlike structure around such nanowire quantum dots by depositing an oxide shell using atomic-layer deposition. Simulations suggest that the intensity collected in our NA=0.6 microscope objective can be increased by a factor 7 with respect to the bare nanowire case. Combining microphotoluminescence, decay time measurements, and numerical simulations, we obtain a fourfold increase in the collected photoluminescence from the quantum dot. We show that this improvement is due to an increase of the quantum-dot emission rate and a redirection of the emitted light. Our ex situ fabrication technique allows a precise and reproducible fabrication on a large scale. Its improved extraction efficiency is compared to state-of-the-art top-down devices.

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Generalized noise terms for the quantized fluctuational electrodynamics: Paper

The quantization of optical fields in vacuum has been known for decades, but extending the field quantization to lossy and dispersive media in nonequilibrium conditions has proven to be complicated due to the position-dependent electric and magnetic responses of the media. In fact, consistent position-dependent quantum models for the photon number in resonant structures have only been formulated very recently and only for dielectric media. Here we present a general position-dependent quantized fluctuational electrodynamics (QFED) formalism that extends the consistent field quantization to describe the photon number also in the presence of magnetic field-matter interactions. It is shown that the magnetic fluctuations provide an additional degree of freedom in media where the magnetic coupling to the field is prominent. Therefore, the field quantization requires an additional independent noise operator that is commuting with the conventional bosonic noise operator describing the polarization current fluctuations in dielectric media. In addition to allowing the detailed description of field fluctuations, our methods provide practical tools for modeling optical energy transfer and the formation of thermal balance in general dielectric and magnetic nanodevices. We use QFED to investigate the magnetic properties of microcavity systems to demonstrate an example geometry in which it is possible to probe fields arising from the electric and magnetic source terms. We show that, as a consequence of the magnetic Purcell effect, the tuning of the position of an emitter layer placed inside a vacuum cavity can make the emissivity of a magnetic emitter to exceed the emissivity of a corresponding electric emitter.
Modeling open nanophotonic systems using the Fourier modal method: Generalization to 3D Cartesian coordinates

Recently, an open geometry Fourier modal method based on a new combination of an open boundary condition and a non-uniform \$k\$-space discretization was introduced for rotationally symmetric structures providing a more efficient approach for modeling nanowires and micropillar cavities [J. Opt. Soc. Am. A33, 1298 (2016)]. Here, we generalize the approach to three-dimensional (3D) Cartesian coordinates allowing for the modeling of rectangular geometries in open space. The open boundary condition is a consequence of having an infinite computational domain described using basis functions that expand the whole space. The strength of the method lies in discretizing the Fourier integrals using a non-uniform circular "dartboard" sampling of the Fourier \$k\$ space. We show that our sampling technique leads to a more accurate description of the continuum of the radiation modes that leak out from the structure. We also compare our approach to conventional discretization with direct and inverse factorization rules commonly used in established Fourier modal methods. We apply our method to a variety of optical waveguide structures and demonstrate that the method leads to a significantly improved convergence enabling more accurate and efficient modeling of open 3D nanophotonic structures.

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BFI (2014): BFI-level 2
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Scopus rating (2013): CiteScore 1.66
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Photon mass drag and the momentum of light in a medium

Conventional theories of electromagnetic waves in a medium assume that the energy propagating with the light pulse in the medium is entirely carried by the field. Thus, the possibility that the optical force field of the light pulse would drive forward an atomic mass density wave (MDW) and the related kinetic and elastic energies is neglected. In this work, we present foundations of a covariant theory of light propagation in a medium by considering a light wave simultaneously with the dynamics of the medium atoms driven by optoelastic forces between the induced dipoles and the electromagnetic field. We show that a light pulse having a total electromagnetic energy \( (h) \) over bar omega propagating in a nondispersive medium transfers a mass equal to \( \delta m = (n^2 - 1) (h) \) over bar omega/c(2)\), where \( n \) is the refractive index. MDW, which carries this mass, consists of atoms, which are more densely spaced inside the light pulse as a result of the field-dipole interaction. We also prove that the transfer of mass with the light pulse, the photon mass drag effect, gives an essential contribution to the total momentum of the light pulse, which becomes equal to the Minkowski momentum \( p(M) = n (h) \) over bar omega/c\). The field's share of the momentum is the Abraham momentum \( p(A) = (h) \) over bar omega/c(2)\), while the difference \( p(M) - p(A) \) is carried by MDW. Due to the coupling of the field and matter, only the total momentum of the light pulse and the transferred mass \( \delta m \) can be directly measured. Thus, our theory gives an unambiguous physical meaning to the Abraham and Minkowski momenta. We also show that to solve the centenary Abraham-Minkowski controversy of the momentum of light in a nondispersive medium in a way that is consistent with Newton's first law, one must account for the mass transfer effect. We derive the photon mass drag effect using two independent but complementary covariant models. In the mass-polariton (MP) quasiparticle approach, we consider the light pulse as a coupled state between the photon and matter, isolated from the rest of the medium. The momentum and the transferred mass of MP follow unambiguously from the Lorentz invariance and the fundamental conservation laws of nature. To enable the calculation of the mass and momentum distribution of a light pulse, we have also generalized the
electrodynamics of continuous media to account for the space- and time-dependent optoelastic dynamics of the medium driven by the field-dipole forces. In this optoelastic continuum dynamics (OCD) approach, we obtain with an appropriate space-time discretization a numerically accurate solution of the Newtonian continuum dynamics of the medium when the light pulse is propagating in it. The OCD simulations of a Gaussian light pulse propagating in a diamond crystal give the same momentum pM and the transferred mass dm for the light pulse as the MP quasiparticle approach. Our simulations also show that, after photon transmission, some nonequilibrium of the mass distribution is left in the medium. Since the elastic forces are included in our simulations on equal footing with the optical forces, our simulations also depict how the mass and thermal equilibria are reestablished by elastic waves. In the relaxation process, a small amount of photon energy is dissipated into lattice heat. We finally discuss a possibility of an optical waveguide setup for experimental measurement of the transferred mass of the light pulse. Our main result that a light pulse is inevitably associated with an experimentally measurable mass is a fundamental change in our understanding of light propagation in a medium.

**General information**

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Organisations: Department of Photonics Engineering, Nanophotonics Theory and Signal Processing, Aalto University  
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Web of Science (2015): Impact factor 2.765  
Web of Science (2015): Indexed yes  
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Web of Science (2014): Indexed yes  
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Scopus rating (2009): SJR 2.469 SNIP 1.346  
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Quantized fluctuational electrodynamics for three-dimensional plasmonic structures

We recently introduced a quantized fluctuational electrodynamics (QFED) formalism that provides a physically insightful definition of an effective position-dependent photon-number operator and the associated ladder operators. However, this far the formalism has been applicable only for the normal incidence of the electromagnetic field in planar structures. In this work, we overcome the main limitation of the one-dimensional QFED formalism by extending the model to three dimensions, allowing us to use the QFED method to study, e.g., plasmonic structures. To demonstrate the benefits of the developed formalism, we apply it to study the local steady-state photon numbers and field temperatures in a light-emitting near-surface InGaN quantum-well structure with a metallic coating supporting surface plasmons.

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Web of Science (2016): Impact factor 3.836
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Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
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Web of Science (2010): Impact factor 3.774
Web of Science (2010): Indexed yes
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Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
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Web of Science (2004): Indexed yes
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Modeling cavities exhibiting strong lateral confinement using open geometry Fourier modal method

We have developed a computationally efficient Fourier-Bessel expansion based open geometry formalism for modeling the optical properties of rotationally symmetric photonic nanostructures. The lateral computation domain is assumed infinite so that no artificial boundary conditions are needed. Instead, the leakage of the modes due to an imperfect field confinement is taken into account by using a basis functions that expand the whole infinite space. The computational efficiency is obtained by using a non-uniform discretization in the frequency space in which the lateral expansion modes are more densely sampled around a geometry specific dominant transverse wavenumber region. We will use the developed approach to investigate the Q factor and mode confinement in cavities where top DBR mirror has small rectangular defect confining the modes laterally on the defect region.

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Open-geometry Fourier modal method: modeling nanophotonic structures in infinite domains

We present an open-geometry Fourier modal method based on a new combination of open boundary conditions and an efficient k-space discretization. The open boundary of the computational domain is obtained using basis functions that expand the whole space, and the integrals subsequently appearing due to the continuous nature of the radiation modes are handled using a discretization based on nonuniform sampling of the k space. We apply the method to a variety of photonic structures and demonstrate that our method leads to significantly improved convergence with respect to the number of degrees of freedom, which may pave the way for more accurate and efficient modeling of open nanophotonic structures.

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Photon momentum and optical forces in cavities

During the past century, the electromagnetic field momentum in material media has been under debate in the Abraham-Minkowski controversy as convincing arguments have been advanced in favor of both the Abraham and Minkowski forms of photon momentum. Here we study the photon momentum and optical forces in cavity structures in the cases of dynamical and steady-state fields. In the description of the single-photon transmission process, we use a field-kinetic one-photon theory. Our model suggests that in the medium photons couple with the induced atomic dipoles forming polariton quasiparticles with the Minkowski form momentum. The Abraham momentum can be associated to the electromagnetic field part of the coupled polariton state. The polariton with the Minkowski momentum is shown to obey the uniform center of mass of energy motion that has previously been interpreted to support only the Abraham momentum. When describing the steady-state nonequilibrium field distributions we use the recently developed quantized fluctuational electrodynamics (QFED) formalism. While allowing detailed studies of light propagation and quantum field fluctuations in interfering...
structures, our methods also provide practical tools for modeling optical energy transfer and the formation of thermal balance in nanodevices as well as studying electromagnetic forces in optomechanical devices.

**Quantum description of light propagation in generalized media**

Linear quantum input-output relation based models are widely applied to describe the light propagation in a lossy medium. The details of the interaction and the associated added noise depend on whether the device is configured to operate as an amplifier or an attenuator. Using the traveling wave (TW) approach, we generalize the linear material model to simultaneously account for both the emission and absorption processes and to have point-wise defined noise field statistics and intensity dependent interaction strengths. Thus, our approach describes the quantum input-output relations of linear media with net attenuation, amplification or transparency without pre-selection of the operation point. The TW approach is then applied to investigate materials at thermal equilibrium, inverted materials, the transparency limit where losses are compensated, and the saturating amplifiers. We also apply the approach to investigate media in nonuniform states which can be e.g. consequences of a temperature gradient over the medium or a position dependent inversion of the amplifier. Furthermore, by using the generalized model we investigate devices with intensity dependent interactions and show how an initial thermal field transforms to a field having coherent statistics due to gain saturation.
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Commutation-relation-preserving ladder operators for propagating optical fields in nonuniform lossy media
We have recently developed a quantized fluctuational electrodynamics (QFED) formalism to describe the quantum aspects of local thermal balance formation and to formulate the electromagnetic field ladder operators so that they no longer exhibit the anomalies reported for resonant structures. Here we show how the QFED can be used to resolve between the left and right propagating fields to bridge the QFED and the quantum optical input-output relations commonly used to describe selected quantum aspects of resonators. The generalized model introduces a density of states concept describing interference effects, which is instrumental in allowing an unambiguous separation of the fields and related quantum operators into left and right propagating parts. In addition to providing insight on the quantum treatment of interference, our results also provide the conclusive resolution of the long-standing enigma of the anomalous commutation relations of partially confined propagating fields.

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Modelling and design of cavities exhibiting high Q and strong mode confinement
Teppo Häyrynen (Invited speaker)
Department of Photonics Engineering
Nanophotonics Theory and Signal Processing

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