Light interaction with nanoresonators: mode volume and quasinormal mode expansion

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Abstract. The most general motion of a system is a superposition of its normal modes, or eigenstates. For Hermitian system, classical normal mode theory applies. For non-Hermitian systems, presently a lot of progress is done to describe the response of optical micro and nanoresonators in their quasinormal mode basis. We have developed a rigorous modal analysis of nanoresonators with unprecedented generality and report numerical results for the general case of 3D resonators, made of dispersive materials on substrate with guiding layers.

1. Introduction

Modes are central in physics, chemistry ... In optics, modes are self-consistent electromagnetic field distributions in waveguides, optical resonators or in free space (plane waves, Hermite–Gaussian modes ...). In waveguide and free space, they are well documented in the literature, as shown by several textbooks on Fourier optics and optical waveguide theory (Vassalo, Snyder & Love, Marcuse, Collin).

We cannot find any textbook on the modal theory of resonators, although nanoresonances play an essential role in current developments in nanophotonics, e.g., optical metasurfaces, integrated optics, optical sensing, photovoltaic devices... The reason is due to mathematical difficulties, see details in the recent review article [1], and especially to the fact that optical resonators are non-Hermitian systems; their physics is not driven by classical normal modes that can be normalized by their energy, but by quasinormal modes (QNMs) with complex frequencies.

In 2013, a general method was proposed to normalize the quasinormal modes of any resonator [1], generalizing earlier works for simple 1D geometries or spheres [2-3]. From that time, the research on the modal theory of resonator has increased at a fast rate. The same year, a freeware was launched [4]. The freeware can be used by any Maxwell equation solver (surface integral methods, volume integral methods, finite element methods, other Fourier expansion, finite element methods with and without PMLs). The only exception seems to be the FDTD method. This year, the first benchmark paper [5] on the computation and normalization of quasinormal modes has been published. The publication, coauthored by 20 researchers from 9 institutions, benchmarks several methods for three geometries of wide interest in modern optics: a two-dimensional plasmonic crystal, a two-dimensional metal grating,
and a three-dimensional nanopatch antenna on a metal substrate. We are close to elaborate standards for the computation of resonance modes. Presently, about 10 theoretical groups in the world are developing a modal theory for analyzing light scattering by resonators, see the recent review article published on the subject that gathers the contribution of all in a comprehensive way [6]. Progress is impressive.

2. Main result
The theory has been reported in a recent paper [7] that we summarize hereafter. Of particular importance in the present context is the successful generalization of the auxiliary-field method, originally proposed for simulating dispersive media with finite difference time-domain simulations [8] and computing the band diagram of dispersive crystals [9], to compute the quasinormal modes of open resonators with finite element methods.

- The quasinormal modes are defined in an extended basis that comprises the electric $E$ and magnetic $H$ fields, like before, but which additionally comprises the polarization $P$ and current $J$ fields. For the first time it is thus the whole resonance eigenstates that are computed: the modes disentangle the resonance associated to the geometry (basically associated to the $E$ and $H$ fields) and the resonance associated to the material (basically associated to the $P$ and $J$ fields).

- This allows us to successfully implement a quasinormal mode solver that efficiently computes the eigenstates of photonic and plasmonic resonators. The associated freeware QNMEig that relies on a COMSOL Multiphysics computational platform can be downloaded on the website of the group.

- On the theoretical side, another important consequence of the auxiliary-field method is a net physical interpretation of temporal dispersion, which lead us to derive orthogonality relations in the augmented formulation for resonances made of dispersive media. Such a derivation that was not possible in earlier works with unspecified dispersion relation [6] leads to the important proposition of closed-form expressions for the eigenstate excitation coefficients.

Figure 1. Ag nanobullet on a Si slab illuminated by a plane wave. More details are found in [7].

Figure 1 shows the results obtained for a silver nanobullet deposited on a Si slab and illuminated from the far-field by a plane wave. It compares the prediction of the far-field and guided-mode radiation diagrams obtained with the freeware and with classical simulations performed with COMSOL. The complexity of the present geometry, unprecedented in modal analysis, is due to the fact that the quasinormal modes not only leak in free space but also in the guided modes of the Si slab. As can be
seen from the figure, when quasinormal modes (QNMs) and PML-modes are included (dashed-black curve), the software accurately predicts the frequency-domain solution of COMSOL (pink). The agreement concerns the far-field radiation diagram in air above and below (left) and the far-field guided-mode radiation diagram (right) in the guided modes of the slab.

Always by using the freeware, we have been able, for the first time for quasinormal mode expansions, to accurately model a situation of quenching, in which a Dirac dipole source emit light in a vicinity of a metallic antenna. Albeit inevitable in plasmonic nanoantennas, quenching has not been previously addressed in the literature on quasinormal mode expansions, and it appears important to see whether it could be modelled. Quenching always occurs at a precise position in a tiny localized volume that strongly depends on the source position, and since quasinormal modes are intrinsic field maps that reflects the symmetry of the geometry and are independent of the source, the modelling of quenching with quasinormal mode expansions represents a serious test, which was successfully completed. Incidentally, the modelling of quenching in the quasinormal mode basis brings us to the important question of the nature of the plasmon modes responsible for quenching, whose answer will cast doubt on the potential of large-\(k\) SPPs.

Unsurprisingly, we find that quenching arises from a mode accumulation at the surface plasma frequency \(\tilde{\omega}_{\text{SP}}\) of large-\(k\) SPPs on flat surfaces, defined by \(\varepsilon_b = -\varepsilon(\tilde{\omega}_{\text{SP}})\). Intuitively, as the separation distance between the dipole and the metal vanishes, the dipole sees a flat interface, and the higher-order plasmons cease to depend on the antenna shape, and resemble those of flat interfaces. The nature of the modes questions the great virtue generally attributed to delocalized SPPs on flat surfaces associated to the flat asymptote in the (complex) \(\tilde{\omega}\) versus (real) \(k\) in all applications related to plasmonic super-resolution and confinement, since their excitation will be inevitably accompanied with quenching. Another related discussion (performed more intuitively) can be found in [10], in relation for a simpler and intuitive geometry, the emission in the vicinity of a flat interface.

3. Conclusion

The modal theory of optical resonators has recently achieved very important improvements, to such an extend that it can be considered as mature nowadays. Refinements are on the road and they can be expected to lead to improved convergence and thus to very powerful numerical tools.

We believe that the joint effort in numerics and theory greatly expands the capabilities of analyzing electromagnetic resonance in nanophotonics, offering increased physical insight and improved computational speed.

With respect to the physics of light interaction with micro and nanoresonators, the new theory that rely on a mathematically-safe normalization of the quasinormal modes leads to a quantitative understanding of how light interact with non-hermitian systems. Many basics can be revisited, sometimes significantly, including the definition of cavity Q’s (please take for a moment a critical view on how to define the energy stored inside a photonic crystal cavity or a nanoantenna) [6] and of the mode volume [1,6,11], an accurate formula for the Purcell effect [1,6], the strong coupling of a quantum emitter and a cavity mode [6], cavity perturbation theory [12,11].

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