Legume: A guided-mode expansion method for photonic crystal slabs for inverse design and light-matter interaction

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***Abstract*— We present a guided-mode expansion (GME) approach – and the corresponding free software named `Legume` – that allows calculating photonic mode dispersion and losses in dielectric photonic crystal slabs, and can be employed for inverse design. We give examples related to (a) symmetry properties and the issue of polarization mixing in coupling to far-field radiation; (b) the occurence of bound states in the continuum (BICs), with very high Q-factors that are accurately calculated by the method; (c) the description of active two-dimensional layers with an excitonic resonance, allowing to describe the regime of strong coupling leading to photonic crystal polaritons.**

Keywords—photonic crystal slabs, guided-mode expansion, exciton-polaritons, inverse design

I. Introduction

Photonic crystal (PhC) slabs, or patterned multilayer waveguides, are known to support truly guided modes with no losses, as well as quasi-guided modes that lie in the continuum of far-field radiation. In this contribution, we present a guided-mode expansion (GME) approach – and the corresponding free software named `legume` – that allows calculating a number of features of PhC slabs: (a) symmetry properties and the issue of polarization mixing in coupling to far-field radiation; (b) the occurence of bound states in a continuum (BICs), which have infinite Q-factor and give rise to topological singularities of the far-field polarization; (c) the description of active two-dimensional layers through a suitably formulated light-matter coupling Hamiltonian, allowing to describe the regime of strong coupling leading to photonic crystal polaritons. Comparison with rigorous coupled-wave analysis (RCWA) is also addressed.

II. Method and Results

The method relies on expanding the magnetic field on the basis of guided modes of an effective homogeneous waveguide with an average dielectric constant in each layer, and diagonalizing the resulting eigenvalue problem. The losses of quasi-guided modes are calculated by photonic perturbation theory and are usually very accurate The `legume` implementation of GME has a backend to the Autograd automatic differentiation library, thereby allowing efficient multiparameter optimization (e.g., complex PhC cavities) and inverse design [1].

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In Fig. 1(a,b) we give an example of photonic mode dispersion and Q-factors for a PhC slab structure that displays several BICs. The quality factors are in very good agreement with the results of RCWA calculations. It should be noticed that the GME method is most accurate when radiative losses are small, i.e., in the high-Q limit.

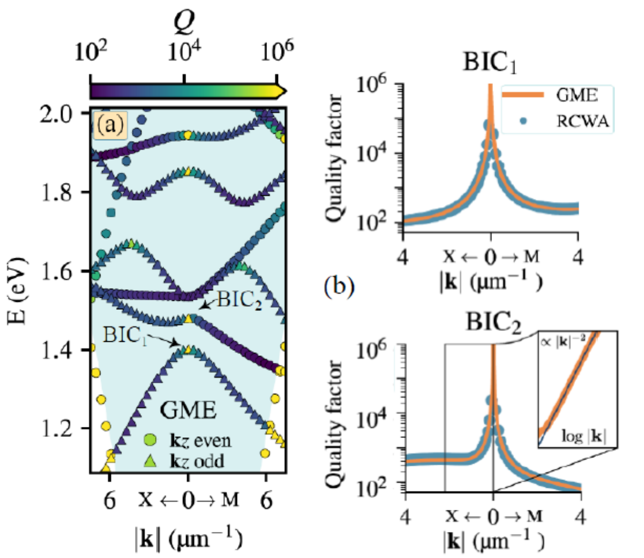

Fig. 1 (a) Dispersion and losses of photonic modes, (b) Q-factor in the proximity of the two BICs indicated in (a), calculated by GME and by RCWA. The PhC slab consists of a square lattice of period a = 400 nm, hole radius r = 100 nm, etched in a suspended slab of thickness d = 80 nm with refractive index n = 3.45.

Exciton-polaritons are calculated by a quantum-mechanical theory, in which the interaction between excitons and photons is treated by diagonalizing a Hopfield-like Hamiltonian in second quantization [2-4]. An example of photonic versus polaritonic dispersion is shown in Fig. 2(a,b). Light-matter interaction leads to anticrossing close to resonance and to hybrid excitations in the strong coupling regime, which inherit the properties of the excitons and photons. In particular, polariton BICs with ultralow radiative losses and with specific topological properties can be described.

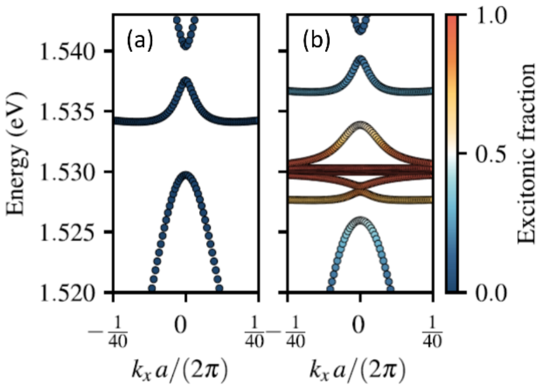

Fig. 2 (a) Dispersion and losses of photonic modes, (b) Q-factor in the proximity of the two BICs indicated in (a), calculated by GME and by RCWA. The PhC slab consists of a square lattice of period a = 400 nm, hole radius r = 100 nm, etched in a suspended slab of thickness d = 80 nm with refractive index n = 3.45.

Thus, the GME method in the `legume` implementation can be exploited for direct and inverse design of advanced nanophotonic structures. The code is freely available on github [6]. Notable features of the last release are the implementation of symmetry with respect to vertical mirror planse, thereby allowing to separate the photonic bands according the polarization, and the explicit inclusion of radiation-matter interaction beyond perturbation theory, leading to photonic crystal polaritons.

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