Stability of bound states in the continuum in low-contrast photonic structures

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Abstract. We consider quality (Q) factor of accidental bound states in the continuum in bilayer resonators consisting of low-index dielectric rods. The dependence of Q factor on the number of periods shows that Q factors increase with the increasing number of rods. We calculated the dependence of the resonator Q factor on the disorder by two methods: analytical (multiple scattering theory) and numerical (finite difference method) and showed that the results are in good agreement. Also, we investigated the dependence of the resonance frequency on disorder.

1. Introduction
Bound states in the continuum (BIC) are resonances with infinite radiative quality (Q) factor [1]. Although infinite Q factor is a mathematical abstraction, high-Q supercavity modes whose nature corresponds to genuine BIC can be excited in real samples [2]. In our work, we consider two types BIC: accidental and symmetry protected [3, 4]. We studied electromagnetic waves in a confined array of rods, which were calculated using the analytical multiple scattering theory (MST) [5, 6]. Also we compared results by MST with numerical simulation by using a finite difference method.

We considered a bilayer structure consisting of a lossless dielectric rods (Fig. 1a) with dielectric permittivity $\varepsilon = 2.1$. The distance between the layers along $y$-axis was $d = 4.7$ cm; the period along $x$-axis was $a = 3$ cm. A point dipole was chosen as the source, which was located at a distance of $3a$ from the left boundary of the structure. The disorder was obtained by randomly changing the coordinates of the rods along $x$-axis. The degree of disorder $\sigma = [0; 0.1]$. For each value of $\sigma$ an ensemble of 100 structures was calculated.

Let us describe the multiple scattering theory by considering two problems in a row. As a first step, we solve the Mie problem for a single particle. Relative to the center of the particle the field can be decomposed into multipoles, which are the product of the exponential function of the angular variable and a Bessel function. Since the field has no singularities at the origin, it can be decomposed into multipoles with the Bessel function of the first kind (since the Neumann functions, i.e. Bessel function of the second kind, and the Hankel functions, i.e. ones of the third kind, have a singularity at zero). The Hankel functions correspond to outgoing cylindrical waves, therefore, the scattered field outside the scatterer region is described by multipoles with the Hankel functions $H^{(1)}(kr)$. The field also has no singularities inside the particle; therefore, it is described by the Bessel functions of the first kind $J(\sqrt{\varepsilon}kr)$. The continuity of the fields
Figure 1. (a) Schematic of bilayer resonator. Red points show periodic structure, black circles show structure with a disorder along the y-axis. (b) The dependence of the Q factor on the rod-pair number of the periodic structure without material losses (solid circles). The dashed line shows the approximation.

Moreover, the larger the particle, the greater the number of multipoles have to be taken into account for sufficient accuracy of the solution of the scattering problem. So, to find scattering on a small particle, it is sufficient to use the Rayleigh approximation, which takes into account only the dipole component of the multipole expansion. For particles comparable to the wavelength, it is often sufficient to consider only 3-5 multipoles.

Next, we move on to the problem with several particles. Let us consider 2 particles for simplicity. The incident field for the first particle consists of the sum of the external incident wave $j_0^1$ and the scattered field on the second particle $h_2$. The difference from the Mie problem considered above is that the scattered field from the second particle is expanded in multipoles centered on the first particle. The corresponding procedure can be written in matrix form:

$$j_1 = j_0^1 + \hat{L}_{21} h_2.$$  \hspace{1cm} (2)

As a result, for each particle there is an equality connecting the amplitude of the incident field and the scattered field. There are two equations with the matrix $\hat{L}$ and the matrix $\hat{T}$, i.e. the number of equations exactly corresponds to the number of unknowns, and the problem can be solved by general linear algebra methods. Note that these self-consistent equations already take into account all the scattering and re-scattering events on all particles, which defines the
name of the strict theory of multiple waves scattering of light. Further, the coupled multipole
method is easily generalized to an arbitrary number of particles.

2. Results
We calculated the transmission spectra by MST for the vicinity of accidental bound state in the
continuum. The obtained spectra were processed and the Q factor was extracted by using the
Fano function fitting. We plotted the dependence of the Q factor on the number of periods N
(Fig. 1b). In the absence of material losses, the Q factor of the BIC increases according to the
cubic law of the number of periods N.

We plotted the dependence of the Q factor on the disorder degree (Fig. 2). The dependence
decreases according to the quadratic law. Multipole scattering theory has some limits with
increasing disorder parameter σ, thus, we compared MST with the finite difference method
that implemented in COMSOL Multiphysics software. The results obtained by MST belong the
confidence interval of the calculations obtained using COMSOL.

![Figure 2. Dependence of Q factor on disorder degree σ. Red circles are simulation by MST and blue circles with confidence intervals by COMSOL.](image)

In addition to our previous work, we calculated the resonance frequency for each disorder
parameter σ and conducted a statistical analysis. The resonant frequency was calculated for
three types of disorder: along the x-, y- and both axes (Fig. 3). Disorder for the other types
was determined similarly to the disorder along the x-axis. In this part, we consider accidental
and symmetry protected BIC.

For both accidental and symmetry protected BIC the average value of the resonance frequency
weakly changes with increasing the disorder degree. Interestingly, that structure with disorder
along the y-axis demonstrates almost a flat frequency dependence. This is associated with
the fact that the symmetry protected BIC emerges at any distances between the layers d and
accidental BIC depends on the rod spacing a only.
Figure 3. Dependence of frequency on the disorder degree $\sigma$ for three types of disorder: along $x$-axis, along $y$-axis, along both axes. (a) accidental BIC, (b) symmetry-protected BIC.

3. Conclusion

Thus, we have shown that the multiple scattering theory and the finite difference method provide equivalent results. The resonant frequencies of both accidental and symmetry protected quasi-BIC in the disordered structure stay almost constant. The weak deviation of the resonant frequency increases with $\sigma$ and that can be explained by decreasing of effective length of the structure in comparison with the ordered one.

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