Optical bistability with bound states in the continuum in dielectric gratings

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We consider light scattering by dielectric gratings supporting optical bound states in the continuum. Due to the presence of instantaneous Kerr nonlinearity the critical field enhancement in the spectral vicinity of the bound state triggers the effect of optical bistability. The onset of bistability is explained theoretically in the framework of the temporal coupled mode theory. As the central result we cast the problem into the form of a singly field-driven nonlinear oscillator. The theoretical results are verified in comparison against full-wave numerical simulations.
Fig. 1: (a) The dielectric grating of Si bars on glass substrate. The plane of incidence $y0z$ is shaded grey. The magenta arrow shows the electric vector of the incident wave. The parameters are $w = 0.5h$, $b = 0.5h$, $L = 1.25h$ (b, c) The electric field profiles of two symmetry protected BICs visualized as $E_x$ in the $y0z$ plane.

I. INTRODUCTION

Engineering high-quality resonances which provide access to tightly localized optical fields has become a topic of paramount importance in electromagnetism\(^1\)\(^-\)\(^4\). In that context, dielectric gratings (DGs) are a useful optical instrument with numerous applications relying on high-quality resonances\(^3\),\(^5\) that occur in the spectral vicinity of the avoided crossings of the DG modes\(^6\). The utmost case of light localization is a bound state in the continuum (BIC) - an embedded state with infinite quality factor coexisting with the scattering solutions\(^4\),\(^7\). Since the seminal paper by Marinica, Borisov, and Shabanov\(^8\) BICs in all-dielectric DGs have been extensively studied both theoretically\(^9\)\(^-\)\(^14\) and experimentally\(^15\),\(^16\). Lately, optical BICs have also been reported in hybrid photonic-plasmonic gratings\(^17\),\(^18\).

The BICs are spectrally surrounded by a leaky band of high-quality resonances which can be excited from the far-zone\(^19\). The excitation of the strong resonances leads to critical field enhancements\(^20\),\(^21\) with the near-field amplitude controlled by the frequency and the angle of incidence of the incoming monochromatic wave. The critical field enhancement allows for activating nonlinear optical effects even with a small amplitude of the incident waves. Such resonant enhancement of nonlinear effects may lead to the effects of symmetry breaking\(^22\) and channel dropping\(^23\).

Among various potential applications in nonlinear optics the BICs have been used for second harmonic (SH) generation. In particular, giant conversion efficiency into SH (up to 40%) was predicted for an array of parallel dielectric cylinders\(^24\). A more practical design of AlGaAs metasurface on a quartz substrate supporting BIC was analyzed in\(^25\), where the efficiency of SH generation $P_{2\omega}/P_{\omega} \sim 10^{-2}$ W is predicted in the vicinity of a BIC. Recently, it was shown theoretically that BIC can enhance the SH conversion efficiency in transition-metal dichalcogenide monolayers by more than four orders of magnitude\(^26\). The BIC is a dark (optically inactive) resonance which cannot be excited from the far field, however, it was shown in\(^27\) that BICs in periodic dielectric structures can be excited by non-linear polarization at the SH frequency induced by the incident field. The same mechanism of destructive interference underlying BICs can result in appearance of high-quality modes in subwavelength dielectric resonators\(^28\),\(^29\), which also demonstrate giant SH generation efficiency\(^30\),\(^31\).

In this paper we consider the effect of the critical field enhancement on optical bistability induced by instantaneous Kerr nonlinearity. Such optical bistability emerges in the scattering spectra in the form of nonlinear Fano resonances\(^32\),\(^33\). Previously the studies of optical bistability with BICs solely relied on either brute force full-wave modelling\(^19\),\(^34\) or phenomenological coupled-mode approach\(^35\). Recently, having considered an array of nonlinear cylinders, we combined the two approaches into a single theory\(^36\) that reduces the problem of finding the nonlinear response to solving a nonlinear coupled-mode equation for a single variable. Herewith all the parameters of the coupled-mode equation are known from solving the linear scattering problem in the spectral vicinity of the BIC which is a far easier task than full-wave modelling of nonlinear Maxwell’s equation. In this paper, we present a generic theory applicable to planar structure with no mirror symmetry with respect to reflection in the plane of the structure. The theory is verified in comparison against full-wave numerical solutions of Maxwell’s equations.
II. BOUND STATES IN THE CONTINUUM

The system under consideration is shown in Fig. 1 (a). It is a dielectric grating assembled of rectangular dielectric bars made of Si. The bars are periodically placed on the glass substrate. Here we only consider the scattering of TE polarized waves with the electric vector aligned with the Si bars as shown in Fig. 1. Under such conditions the propagation of electromagnetic waves is controlled by the Helmholtz equation for the $x$ component of the electric field

$$\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)E_x + k^2[n_0^2 + 2n_0n_2|E_x|^2]E_x = 0,$$

(1)

where $k$ is the vacuum wavenumber, and $n_{0,2}$ are linear and nonlinear refractive indices, correspondingly. In what follows the refractive index of Si is taken as $n_0 = 3.575$, while the refractive index of the substrate $n_0 = 1.5$.

Our numerical simulations with the use of Dirichlet-to-Neumann map method have demonstrated that for the set of parameters specified in the caption to Fig. 1 the system supports two in-Γ BICs coexisting with the zeroth diffraction order. The eigenmode profiles of the BICs are shown in Fig. 1 (b) and Fig. 1 (c). Notice the striking difference between BIC 1 and BIC 2 in Fig. 1 (b) and Fig. 1 (c): the field of BIC 1 is mostly localized in the Si bars, whereas the field of BIC 2 is spread across the whole grating. This difference is due to the higher eigenfrequency of BIC 2 allowing the first diffraction order in the glass substrate.

One important property of the BICs is the emergence of a collapsing Fano feature in its parametric vicinity. In this paper, we consider light scattering near the normal incidence so that the incident light couples to the band of resonant modes with diverging $Q$-factor as $\theta \to 0$. In Fig. 2 (a) and Fig. 2 (b) we show the transmittance spectra in the spectral vicinity of BIC 1 and BIC 2, correspondingly. One can see that in both cases one observes a narrow Fano feature which collapses at the exact normal incidence. This difference is due to the higher eigenfrequency of BIC 2 allowing the first diffraction order in the glass substrate.

One can see from Fig. 2 that BIC 1 occurs as an isolated resonance, while BIC 2 emerges as a result of hybridisation of two resonant modes with one of them acquiring infinite life-time. The latter mechanism of BIC has been previously demonstrated for dielectric gratings. In the next section we provide a theoretical description of the line shapes of the Fano anomalies induced by the BICs extended to the effects of Kerr nonlinearity triggered by critical field enhancement.

III. SCATTERING THEORY

The aim of this section is to formulate the equation for the amplitude of the quasi-BIC resonant mode in the framework of the temporal coupled mode theory (TCMT). The generic case of a TCMT applied to a 2D structure...
is considered in\(^{44}\). It has been demonstrated that in the absence of mirror symmetry with respect to \(y \rightarrow -y\) the application of TCMT requires considering four scattering channels. However, as the above symmetry holds in our case, we shall apply a two-channel TCMT in this paper. Following\(^{36}\) we only consider the effect of a single resonant mode mentioning in passing that a generalization of the TCMT to multimodal case is possible\(^{45}\).

### A. Coupled mode approach

Let us start with the TCMT equation for an isolated resonance\(^{43}\)

\[
\frac{da(t)}{dt} = i(\omega_0 - \Gamma)a + (d^*|s^{(+)}) ,
\]

where \(a(t)\) is the time-dependent amplitude of the resonant mode, \(\omega_0\) is the resonant frequency, \(\Gamma\) is the inverse life-time of the resonance, \(|d\rangle\) is the vectors of coupling constants to the scattering channels, and \(|s^{(+)})\) is the vector of incident amplitudes. Since we stay in the domain where only specular reflection is allowed, both \(|s^{(+)}) = (s^{(+)}_1, s^{(+)}_2)^T\) are \(2 \times 1\) vectors. The subscripts \(1, 2\) are applied to the upper and lower half-spaces, correspondingly.

Let us, e.g., assume that a monochromatic plane wave with frequency \(\omega\) is incident onto the grating from the upper half-space. The vector of the incident amplitudes is written as

\[
|s^{(+)}) = \begin{pmatrix} \sqrt{I_0} & 0 \end{pmatrix}^T ,
\]

where \(I_0\) is the flux density supported by the incident wave. After the time-harmonic substitution \(a(t) = ae^{i\omega t}\) one finds

\[
a = \frac{d_1\sqrt{I_0}}{i(\omega - \omega_0) + \Gamma} .
\]

Finally, the outgoing amplitudes can be found from the following equation

\[
|s^{(-)}) = \hat{C} + a|d\rangle .
\]

Here, \(\hat{C}\) is the matrix of direct (non-resonant) process. In the case of the symmetry protected BIC, the matrix \(\hat{C}\) can be easily obtained numerically by solving the scattering problem at the normal incidence with the incident frequency equal to the BIC frequency. In the other words exactly in the point of the Fano resonance collapse\(^{36}\).

The general solution of the linear scattering problem can be written through the scattering matrix \(\hat{S}(\omega)\) which links the vectors of incident and outgoing amplitudes

\[
|s^{(-)}) = \hat{S}(\omega)|s^{(+)})\]

Since the system under consideration is both energy preserving and symmetric with respect to time reversal, the matrices \(\hat{S}(\omega)\) and \(\hat{C}\) are simultaneously unitary and symmetric\(^{46}\). The most generic form of \(\hat{C}\) can be parameterized in the following manner

\[
\hat{C} = e^{i\phi} \begin{pmatrix} \rho e^{-i\eta} & i\tau \\ i\tau & \rho e^{i\eta} \end{pmatrix} ,
\]

where the real valued \(\rho\) and \(\tau\) are the absolute values of the reflection and transmission amplitudes which have to satisfy the following equation

\[
\rho^2 + \tau^2 = 1.
\]

Thus, taking the above into account we are left with only three independent parameters, \(\theta, \eta,\) and \(\rho\) which can be analytically derived from Eq. \(^{7}\).

The quantities \(\hat{C}\) and \(|d\rangle\) are linked through the following equation\(^{43}\)

\[
\hat{C}|d^\star\rangle = -|d\rangle,
\]

which is a consequence of both energy conservation and time-reversal symmetry. Equation \(^{9}\) constitutes a homogeneous algebraic equation for unknown \(|d\rangle\). Since the complex conjugation is involved in Eq. \(^{9}\) it has to be solved for
four independent variables, i.e. the real and imaginary parts of $|d\rangle$. This results in a system of four equation of rank 2. Therefore the general solution of Eq. (10) can be written as a function of two independent parameters $\alpha$ and $\beta$.

$$ |d\rangle = \begin{pmatrix} (\tau \alpha - i(1 + \rho)\beta)e^{i\frac{2\pi}{2\tau}} \\ (\tau \beta - i(1 + \rho)\alpha)e^{i\frac{2\pi}{2\tau}} \end{pmatrix}. \quad (10) $$

Notice that in general $d_1 \neq d_2$. Thus, Eq. (10) takes into account the asymmetry of the coupling to the upper and lower half-spaces due to the lack of mirror symmetry in the plane of the structure, see Fig. 1 (a).

Another important relationship is a consequence of energy conservation

$$ 2\Gamma = \langle d|d\rangle. \quad (11) $$

The above equation is derived by considering the decay dynamics of the system with no impinging wave. Assume that a certain amount of energy $E$ is load into the resonant mode, then the solution of Eq. (2) $a(t) = a(0)e^{i\omega_0t-\Gamma t}$. Given that the eigenmode stores a unit energy, the energy dissipation rate can be found as

$$ \frac{dE}{dt} = -2\Gamma|a_0|^2, \quad (12) $$

where $E$ is the energy stored in the resonant eigenmode. On the other hand if each scattering channel attenuates a unit of energy per unit of time, Eq. (8) yields

$$ \frac{dE}{dt} = -\langle d|d\rangle|a_0|^2. \quad (13) $$

Combining Eqs. (12) and (13) we find Eq. (11). Notice, that normalization of both the eigenmode and decay channels is important for deriving Eq. (11). Application of Eq. (11) to Eq. (10) yields

$$ \alpha^2 + \beta^2 = \frac{2\Gamma}{\tau^2 + (1 + \rho)^2}. \quad (14) $$

Let us summarize the findings of this subsection. First, as it is seen from Eq. (4) the resonant response is due to vanishing $\Gamma$ in denominator. Notice that both $\Gamma$ and $\omega_0$ are known from the eigenmode spectrum of the grating, they can be determined as the real and imaginary part of the resonant frequency of the leaky band host the BIC, as it has been done in Ref. 36. Second, the coupling vector $|d\rangle$ is defined from the matrix of the direct process Eq. (7) via Eq. (10) up to two unknown real-valued parameters. Quite remarkable is that the presence of a symmetry protected BIC gives an easy access to the the matrix of the direct process by simply computing the scattering solution at the BIC frequency and the normal incidence. Finally, Eq. (14) allows for eliminating of one of the free parameters, say $\alpha$ in Eq. (10). The remaining parameter $\beta$ can be found by easily found by fitting the transmittance spectrum found through the full-wave solution of the scattering problem.

### B. Green’s function

Let us now generalize the above result to the system with Kerr nonlinearity. In this subsection we apply the resonant state expansion method for deriving the TCMT equation with account of nonlinearity. The key figure of merit in the resonant state expansion method is Green’s function of Maxwell’s equations. According to Eq. (15) the spectral representation of Green’s function can be written as

$$ G(r', r, k_0, k_y) = \frac{\sum_{n} E_{x}^{(n)}(r, k_y)E_{x}^{(n)}(r', -k_y)}{2k[k - k_n(k_y)]}. \quad (15) $$

where $E_{x}^{(n)}(r, k_y)$ the field profile of the $n_{th}$ resonant eigenmode and $k_n(k_y)$ is the dispersion of the resonant eigenfrequency of the leaky band in terms of vacuum wave number, $k = \omega/c$ with $c$ as the speed of light. The symbol $\sum_n$ is used for the combined contribution of a discrete sum and integration along the cuts. For the spectral representation Eq. (15) to be valid the eigenfields $E_{x}^{(n)}(r, k_y)$ must obey the following normalization condition

$$ 1 + \delta_{0,k_n} = I_n^V + \lim_{k \to k_n} \frac{S_n^{OV}}{k^2 - k_n^2}. \quad (16) $$
with

\[ I_{n}^{V} = \int_{V} dV E_{x}^{(n)}(r, -k_{y})E_{x}^{(n)}(r', k_{y}) \tag{17} \]

and

\[ S_{n}^{ov} = \oint_{\partial V} dS \left[ E_{x}^{(n)}(r, -k_{y})\partial_{S}E_{x}^{(n)}(r', k_{y}, k) - E_{x}^{(n)}(r, -k_{y}, k)\partial_{S}E_{x}^{(n)}(r', k_{y}) \right], \tag{18} \]

where \( \partial_{S} \) is used for the normal derivative with respect to the boundary of the elementary cell and \( \tilde{E}_{x}^{(n)}(r', k_{y}, k_{0}) \) is the analytic continuation of the eigenfield in the vicinity of its resonant eigenfrequency such as

\[ E_{x}^{(n)}(r', k_{y}) = \lim_{k \to k_{n}} \tilde{E}_{x}^{(n)}(r', k_{y}, k). \tag{19} \]

### C. Resonant approximation

To establish a link between the resonant state expansion and the single mode TCMT we apply resonant approximation, i.e. in Eq. (15) we retain only the term with \( k - k_{n}(k_{y}) \) in the denominator. All the other terms are assumed to be independent of frequency on the scale of the narrow Fano feature induced by the BIC. In terms of the TCMT the non-resonant terms are accumulated into the direct process. The resulting resonant Green’s function is simply

\[ G^{(res)}(r', r) = \frac{E_{x}^{(o)}(r, k_{y})E_{x}^{(o)}(r', -k_{y})}{2k[k - k(k_{x})]}, \tag{20} \]

where \( E_{x}^{(o)}(r, k_{y}) \) is the profile of the resonant eigenmode. Above we omitted the band index of the dispersion \( k(k_{x}) \) bearing in mind that the resonant approximation uses the dispersion and the mode profiles of the BIC host band.

At first let us again consider linear scattering problem. As before we assume that a TE polarized plane wave with intensity \( I_{0} \) impinges onto the structure at the near normal incidence. Then, solving Eq. (11) with the resonant Green’s function Eq. (20) one finds

\[ E_{x} = \frac{\sqrt{I_{0}E_{x}^{(o)}(r, k_{y})}}{2k[k - k(k_{x})]} \int_{V} dV E_{x}^{(o)}(r', -k_{y})J(r'), \tag{21} \]

where the source term can be express through the incident field \( E_{x}^{(in)} \) as

\[ J = -\left( \frac{\partial^{2}}{\partial y^{2}} + \frac{\partial^{2}}{\partial z^{2}} \right) E_{x}^{(in)} - n_{0}^{2}E_{x}^{(in)}, \tag{22} \]

where \( E_{x}^{(in)} \) is normalized to carry a unit of energy per unit of time per unit area of the boundary of the scattering domain. Thus, amplitude of the physical incident wave is only controlled by \( I_{0} \).

To be consistent with the resonant approximation we also assume that the near-field response is dominated by the quasi-BIC eigenmode

\[ E_{x} = \frac{1}{\sqrt{A}} a E_{x}^{(o)}, \tag{23} \]

where \( A \) is the normalization constant. Substituting the above equation into Eq. (21) one finds

\[ a = \frac{\sqrt{I_{0}A}}{2k[k - k(k_{x})]} \int_{V} dV E_{x}^{(o)}(r', -k_{y})J(r'). \tag{24} \]

By comparing Eqs. (21) and (24) one finds

\[ d_{1} = \frac{i\sqrt{Ac}}{2k} \int_{V} dV E_{x}^{(o)}(r', -k_{y})J(r'), \tag{25} \]

where \( c \) is the speed of light. The above equation is difficult to be applied in computations, since it requires the explicit analytic form of the leaky mode profiles under normalization condition Eq. (16). We, however, already know from the previous subsection how \( d_{1} \) can be found from the scattering spectra with the use of Eqs. (10) and (14).
D. Nonlinear case

Now let us generalize the above result onto the non-linear case. After taking the same route we end up with the following equation for \( a \)

\[
a + J = \frac{n_0 n_2 k}{A[k - k(k_y)]} |a|^2 a = \frac{\sqrt{I_0} d_1}{i c [k - k(k_y)]},
\]

(26)

where

\[
J = \int_{V_{\text{lin}}} dV \left| E_x^{(0)}(-k_y)E_x^{(0)}(k_y)\right|^2,
\]

(27)

and the integration is performed only over the domain with nonlinear refractive index \( V_{\text{lin}} \). Finally notice that \( J \) must be parabolic in \( k_y \), since the problem is symmetric with respect to the angle of incidence. Therefore we drop the dependence on \( k_y \) using the field profile in the \( \Gamma \)-point, i.e. the BIC

\[
J = \int_{V_{\text{lin}}} dV |E_x^{(\text{BIC})}|^4 + \mathcal{O}(k_y^2).
\]

(28)

Since the BIC profile is a well behaved function decaying with the distance from the grating. Following one easily finds that Eq. (26) is equivalent to the integration over \( z \) from plus to minus infinity

\[
1 = \int_{-\infty}^{\infty} dV n_0^2 |E_x^{(\text{BIC})}|^2.
\]

(29)

Important, Eq. (29) does not contain surface terms and, thus, can be easily implemented in simulations taking into account that the BIC decays exponentially with \(|z| \to \infty \). Finally, notice that the integral in Eq. (28) is equal to twice electromagnetic energy stored in the BIC. Thus, to be consistent with Eq. (11) we set \( A = 2 \).

E. Nonlinear temporal coupled mode equation

Now, in accordance with Eq. (26) the final result reads

\[
[i(\omega - \omega_0) + \Gamma]a + iJ n_0 n_2 |a|^2 a = \sqrt{I_0} d_1.
\]

(30)

Equation (30) only differs from Eq. (4) by the presence of nonlinear term proportional to \( J \). It means that for describing the nonlinear response in the spectral vicinity of a BIC it is sufficiently to know the solution of the linear problem including the field profile of the BIC. Once the BIC field profile is known it can be substituted into Eq. (28) to find \( J \). The nonlinear Eq. (30) can be then solved for the response in the frequency domain.

It is remarkable that the nonlinear correction in Eq. (30) exactly coincides with that obtained previously with the perturbation theory\(^{49}\). Notice, however, that the results reported in\(^{49}\) have been obtained under assumption of smallness of the nonlinear term. Another issue with straightforward application of the perturbation theory is the normalization condition of the unperturbed eigenmodes. The formal solution presented in\(^{49}\) involves integration across the whole space which is impossible due to divergence of the resonant eigenmodes in the far zone\(^{50}\). As one can see from the previous subsection the normalization issue can only be easily resolved in the spectral vicinity of a BIC.

Finally, in the time domain Eq. (30) can be replaced by

\[
\frac{d}{dt} \left( a + J n_0 n_2 |a|^2 a \right) = (i\omega_0 - \Gamma) a + \sqrt{I_0} d_1 e^{i\omega t}.
\]

(31)

The time-harmonic solutions of the above equations can be tested for stability by series expansions with respect to small perturbation as explained in\(^{36}\).

IV. NUMERICAL VALIDATION

In this section we apply our previous findings to the scattering spectra. To obtain the matrices of the direct process we numerically solved the linear scattering problem at exact normal incidence with the vacuum wave number of the
The thin magenta lines demonstrate Fano resonances unperturbed by the nonlinearity. The blue dots are full-wave numerical solutions obtained with pseudospectral method. The stable solutions of Eq. (30) are shown by thick grey lines. Thin red lines show unstable solutions of Eq. (30). Dashed black line in (c) show the transmittance at exact normal incidence.

In the next step the numerical values of the three remaining parameters \( \omega_0 \), \( \Gamma \), and \( \alpha \) were evaluated by fitting to the scattering spectra in Fig. 2 at different angles of incidence. The effective nonlinearity coefficient was found with Eq. (28) by integrating the BIC profiles shown in Fig. 1 (b), and Fig. 1 (c). The results are collected in Table 1. In Table 1 we also present the ratio of the absolute values of the coupling constants \( d_1 \) and \( d_2 \). One can see that in both cases the coupling to the lower half-space is somewhat larger than to the upper half-space, \( |d_1| < |d_2| \).

| \( \theta \) | \( h\omega_0/c \) | \( h\Gamma/c \) | \( \alpha \) (p.d.u.) | \( |d_1/d_2| \) | \( J \) (p.d.u.) |
|---|---|---|---|---|---|
| BIC 1 | 1° | 2.5670 | 0.065 \cdot 10^{-5} | 6.24 \cdot 10^{-3} | 0.097 | 3.04 \cdot 10^{-2} |
| BIC 1 | 2° | 2.5689 | 0.031 \cdot 10^{-3} | 1.23 \cdot 10^{-2} | 0.914 | 3.04 \cdot 10^{-2} |
| BIC 2 | 0.2° | 4.39074 | 1.59 \cdot 10^{-3} | 9.05 \cdot 10^{-2} | 0.717 | 3.79 \cdot 10^{-4} |

To obtain the nonlinear scattering spectra Eq. (1) was solved numerically with the pseudospectral method\(^{51}\). In our simulations we took \( n_2 = 5 \cdot 10^{-18} \text{ m}^2/\text{W} \) which corresponds to silicon at 1.8 \( \mu \)m.\(^{52}\) The results are plotted in Fig. 3 in comparison with numerical solution of Eq. (30). The intensities of the incident waves are given in the caption to Fig. 3. First of all one can see in Fig. 3(a) and Fig. 3(b) that there is a reasonably good agreement between the TCM and the full-wave spectra for BIC 1. The agreement can be made perfect by slightly tuning \( \alpha \) and/or \( J \). For BIC 2, however, the agreement is not that good and our theory can only provide a rough estimate of the parameter values leading to optical bistability. The discrepancy is due to the single-mode approximation which is not capable to account for all features of the BIC emerging with an avoided crossing. To highlight the limitations of the single-mode approximation, we plot the numerical results with the pseudospectral method for BIC 1 at different angles of incidence in Fig. 3(a) and Fig. 3(b). The blue dots are full-wave numerical solutions obtained with pseudospectral method. The stable solutions of Eq. (30) are shown by thick grey lines. Thin red lines show unstable solutions of Eq. (30). Dashed black line in (c) show the transmittance at exact normal incidence.
TCMT in Fig. 3 (c) we plotted the transmittance at the normal incidence. One can easily see that the transmittance at the normal incidence is dependent on frequency, whereas the single-mode TCMT assumes that it is constant. On the other hand, even the single-mode approximation manages to grasp the major feature of BIC 2 with respect to initiating bistability. One can see from Table 1 that the effective nonlinearity coefficient $J$ is two orders of magnitude smaller with BIC 2 than with BIC 1. The reason for this is clearly seen from Fig. 1 (b) and Fig. 1 (c) - the field of BIC 1 is concentrated about the nonlinear medium (silicon bars), while for BIC 2 the field is evenly spread across the whole grating. The small value of $J$ results in very high intensities needed to trigger optical bistability. This rules out application of BIC 2 in a realistic experiment.

V. SUMMARY AND CONCLUSIONS

In this paper we considered the effect of optical bistability induced by bound states in the continuum (BICs) in dielectric gratings. We proposed a coupled mode approach which leads to a single nonlinear equation for the amplitude of the resonant eigenmode of the BICs host band. It is shown how all parameters entering the nonlinear coupled mode equation can be evaluated from the solution of the linear scattering problem.

We believe that the approach presented here can be of use in engineering photonic systems with the resonantly enhanced nonlinear response, as the coupled mode equation is much easier to get solved than nonlinear Maxwell’s equations. At the same time our approach gives a cue for choosing the type of BICs in order to maximize the nonlinear effect. Namely, it has been shown that the BIC with the frequency lower than the first diffraction order in the substrate are better in activating the nonlinearity.

On the other hand, from the fundamental view point we have seen that the scattering of light in the spectral vicinity of a BIC can be handled by the resonant state expansion method. This naturally prompts us to extend the theory for the two-mode case which potentially leads to an intricate interplay between the BICs and the other mode with a finite live-time that can be excited from the far zone even at the normal incidence. The application of resonant state expansion to finite-lived states would, however, require introducing the analytical continuation normalization condition, Eq. 19 to eigenmodes that are known only numerically. We speculate that the above problem can be an interesting topic for future studies.

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