Multipolar origin of bound states in the continuum

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We suggest a novel approach to explain the physics of bound photonic states embedded into the radiation continuum. We study dielectric metasurfaces composed of planar periodic arrays of Mie-resonant nanoparticles (“meta-atoms”) which support both symmetry protected and accidental bound states in the continuum, and employ the multipole decomposition approach to reveal the physical mechanism of the formation of such nonradiating states in terms of multipolar modes generated by isolated meta-atoms. Based on the symmetry of the vector spherical harmonics, we identify the conditions for the existence of bound states in the continuum originating from the symmetries of both the lattice and the unit cell. Using this formalism we predict that metasurfaces with strongly suppressed spatial dispersion can support the bound states in the continuum with the wavevectors forming a line in the reciprocal space. Our results provide a new way for designing high-quality resonant photonic systems based on the physics of bound states in the continuum.

I. INTRODUCTION

The quest for compact photonic systems with high quality factor (Q factor) modes led to the rapid development of optical bound states in the continuum (BICs). BICs are non-radiating states, characterized by the resonant frequencies embedded to the continuum spectrum of radiating modes of the surrounding space [1, 2]. The BICs first appeared as a mathematical curiosity in quantum mechanics [3]. The discovery of BICs in optics immediately attracted broad attention (see, e.g., Refs. [4–6]) due to high potential in applications in communications [7, 8], lasing [9–12], filtering [13], and sensing [14–16]. Recent achievements in the field of BIC are discussed in Refs. [17–26].

Decoupling of the resonant mode from the radiative spectrum, which is the basic idea behind the BIC, can be interpreted in several equivalent ways. Within the coupled-mode theory, it corresponds to nullifying the coupling coefficient between the resonant mode and all radiation channels of the surrounding space [27]. Alternatively, the appearance of BICs is explained as vanishing of Fourier coefficients corresponding to open diffraction channels due to the symmetry of the photonic structure. At the particular high-symmetry points of the reciprocal space, for example, at the Γ point, the continuous spectrum is divided into the modes of different symmetry classes with respect to the reflectional and rotational symmetry of the photonic system. The bound states of one symmetry class can be found embedded in the continuum of another symmetry class, and their coupling is forbidden as long as the symmetry is preserved. Such kind of BIC is called symmetry-protected, and they also allow interpretation in terms of topological charges defined by the number of times the polarization vectors winds around the BICs presented as vortex centers in the polarization field [28]. In contrast to the symmetry-protected BIC, the so-called accidental BICs [1, 28–31] can be observed out of the Γ-point due to an accidental nulling of the Fourier (coupling) coefficients via fine tuning of parameters of the photonic system. Such a mechanism is also known as Friedrich-Wintgen scenario [32].

Despite the number of existing approaches to understand the nature of BICs, there is still a room for further
development of the theory. During the previous few years
the electromagnetic multipole theory [33] has been exten-
sively developed as a natural tool of nanophotonics deal-
ing with the lowest (fundamental) resonances of the sys-
tem. The main advantage of the multipole decomposition
method (MDM) is that it provides a representation of an
arbitrary field distribution as a superposition of the fields
created by a set of multipoles [34, 35]. Namely, the mul-
tipole expansion has been widely used to determine the
polarization and directivity patterns of the scattered field
of single particles and their clusters both plasmonic and
dielectric [34, 36] for a variety of applications such as po-
larization control device [35], dielectric nanoantenna [37],
light demultiplexing [38], and others. A number of novel
optical phenomena have been explained within the MDM
such as anapole effect [39, 40], optomechanical phenom-
ena [41, 42], and Kerker effect [43, 44].

In this work, we extend the MDM approach for ex-
plaining both symmetry protected and accidental BICs.
We provide a theory of BICs origin in terms of MDM for a
general case of any periodic structure and develop an an-
alytical method, which determines the contribution of the
vector spherical harmonics to the far field (Section II).

In the vector spherical harmonics (VSH) ba-
sis, we take the advantage of the internal symmetry and
provide the group-symmetry approach to identifying the
BIC formation in terms of the unit cell and lattice sym-
metries (Section III). We implement field multipole ex-
pansion of the eigenmodes of a periodic two-dimensional
(2D) photonic structure supporting BIC. We illustrate the
developed technique by considering a 2D square array
of spheres and extending it to the case of a photonic crys-
tal slab with a 2D array of cylindrical holes (Section IV).

The developed approach can be easily extended even fur-
ther to periodic structures with other types of the unit
cell and other lattice symmetries. The proposed method
both provides a deeper understanding of the photonic
BIC physics and gives a tool for an effective designing of
high-Q resonant photonic systems.

II. MULTIPOLAR APPROACH

In this section we consider the modes of a two-
dimensional periodic array of dielectric nanoparticles
with arbitrary shape (see Fig. 1), and obtain an expres-
sion connecting the multipolar content of the field inside
and outside the nanoparticles. We denote the VSH as
$\mathbf{M}_{p,m,n}(k, \mathbf{r})$ (magnetic) and $\mathbf{N}_{p,m,n}(k, \mathbf{r})$ (electric)
relaying on the definition presented in Ref. 45. We intro-
duce an additional notation $\mathbf{W}_{p,m,n}(k, \mathbf{r})$, for both types of
VSHs, where inversion parity index $p_1 = (-1)^{n+1}$ for
$\mathbf{M}_{p,m,n}(k, \mathbf{r})$, and $p_1 = (-1)^n$ for $\mathbf{N}_{p,m,n}(k, \mathbf{r})$. Index $n$
is the multipole order, $m$ is from 0 to $n$, and $p_r = 1$
if $\mathbf{W}_{p,m,n}$ is even under reflection from $y = 0$ plane
($\varphi \rightarrow -\varphi$ in the spherical system), and $p_r = -1$ if it is
odd [46].

In homogeneous medium with permittivity $\varepsilon$, any solu-
tion of the Helmholtz equation with wavevector $k = \sqrt{\varepsilon \omega}$
can be expanded in terms of these functions [47]. The
field inside of $j$-th cell of the array $\mathbf{E}^{in}$ can be written in terms of multipolar decomposition:

$$\mathbf{E}^{in}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \sum_{p_r} \mathbf{E}_0 \mathbf{D}_{p_r,m,n}(k_2, \mathbf{r'}) e^{i(k_0 \cdot \mathbf{r}_j)},$$

where $k_2 = \sqrt{\varepsilon_2 \omega}$ is the wavevector in the material, the
superscript (1) stands for spherical Bessel functions in the
radial part of the VSH, $k_0$ is the Bloch vector, $\mathbf{r'} = \mathbf{r} - \mathbf{r}_j$, and $\mathbf{r}_j$ is the position of a single sphere (see Fig. 1).

$D_{p_r,m,n}$ are the coefficients of the multipolar decompo-
sition, which will be discussed in Section III. In similar
manner, the field outside the array is expressed as follows (see Appendix B):

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0 \sum_{p_k, p_r,m,n} \mathbf{D}_{p_k,m,n}(k_1) \times$$

$$\times \int \int dk_x dk_y \delta(\mathbf{k}_x - \mathbf{k}_y) \delta(\mathbf{k}_y - \mathbf{k}) e^{i\mathbf{k}_r} \left[ \mathbf{Y}_{p_k,m,n} \left( \frac{\mathbf{k}}{|\mathbf{k}|} \right) \right].$$

(2)

Here $\mathbf{K}$ is the reciprocal lattice vector, $k_z = \pm \sqrt{k_x^2 - k_y^2}$,
$|\mathbf{k}| = k_1 = \sqrt{\varepsilon_1 \omega}$, $V_i$ is the volume of the first Brillouin
zone. The spherical vector functions $\mathbf{Y}(\mathbf{n})$ depend on the
spherical coordinates of a unity vector $\mathbf{n}$ and they are
given in the Appendix A. Their symmetry coincides with the symmetry of $\mathbf{W}$-function with the identical in-
dices. The relation between $D$ and $\mathbf{D}$ is discussed in
Appendix C, and for the case of an array of spherical
particles, coefficients $\mathbf{D}$ can be derived analytically.

The summation in Eq. (2) over the reciprocal vectors
corresponding to open diffraction channels, i.e. the terms
with real $k_z$, provides the contribution into the far field.
The BIC appears at the frequencies below the diffraction
limit, thus, only the zero-order term with $\mathbf{K} = 0$ gives
non-zero contribution to the far field:

$$\mathbf{E}(\mathbf{r}) = \frac{E_0 V_b}{2\pi k_1 k_1} e^{i\mathbf{k}_r} \sum_{p_k, p_r,m,n} i^{-n} \mathbf{D}_{p_k,m,n}(k_1) \left[ \mathbf{Y}_{p_k,m,n} \left( \frac{k_1}{k_1} \right) \right],$$

(3)

where $|\mathbf{k}_1| = k_b$, and $k_{1z} = \pm \sqrt{k_x^2 - k_y^2}$. According to
Eq. (3), the contribution of the multipole with numbers
$p_k, p_r, m, n$ into the far field in the direction defined by the
wave vector $\mathbf{k}_1$ is proportional to the multipole ex-
pansion coefficient $\mathbf{D}$ and the value of spherical vector
function $\mathbf{Y}$ in the given direction. The Eq. (3) provides the correspondence between the radiation pattern of a
single unit cell and the far-field properties of the whole
infinite array allowing for interpolating the BIC in terms of
MDM. In strong contrast to a single nanoparticle, where
each multipole contributes to the far field, in case of a
subdiffractive array there might be direction, where non of the multipole gives any contribution, or alternatively the non-zero contribution of different terms may eventually sum up to zero. The formulated alternative gives a sharp distinction between the symmetry protected and accidental BIC.

At-Γ point BIC. The Γ-point BIC corresponds to the absence of the far-field radiation in the direction along the z-axis. Due to the structure of VSH, it appears that a number of multipoles do not radiate in the vertical direction along the z-axis. If the field inside a single unit cell consists only of such multipoles, there will be no total radiation in z-direction. This simple fact is illustrated in the upper panel in Fig. 1(b). Noticing that only \( Y_{p,p-1} \) functions with \( m=1 \) are non-zero in parallel to the z-axis direction, we can conclude that at the Γ-point in the subdiffractive array all the modes which do not contain the harmonics with \( m = 1 \) are symmetry-protected BICs. This fundamental conclusion lies in the basis of recent experimental demonstration [9] of lasing with BIC in a 2D subdiffractive array of nanoparticles. The particular operational mode consisted of vertical dipoles oriented along the z-axis, thus, not contributing into the only open channel. There exist an approach [1, 28] that the eigenmodes at the Γ-point can radiate in the normal direction \( z \) if their fields are odd under \( C_{2z} \) rotations, and do not have any other rotational symmetry of \( C_{nz} \)-type. In terms of multipole moments, this follows from the fact that at the Γ-point any radiative mode should contain multipoles with \( m = 1 \). On the other hand, in virtue of the symmetry, the even modes have zero radiation losses, i.e. infinite radiation quality factor, which are known as symmetry-protected BICs.

Off-Γ BIC. Let us now turn to the case of accidental BIC description. In general case, coefficients \( D \) are complex numbers. They define the amplitudes and phase delay between the multipoles. However, in accordance with [29], if the structure has time reversal and inversion symmetry, the eigenmodes must satisfy the condition \( E(r) = E^*(−r) \). This fact imposes strict conditions on the multipoles’ phases, because some of them are even under inversion and some of them are odd, the coefficient \( D_{-1p, mn} \) before the odd ones must be imaginary. It follows that every term of the sum in Eq. (3) is purely real, and all multipoles are in-phase or anti-phase. All coefficients depend on \( k \)-vector and structure’s parameters and in a case of the off-Γ BICs this sum turns to zero. In other words, for the particular \( k_1 \) all vector harmonics add up to zero in the direction of \( k_1 \), analogously to the anti-Kerker effect, because they are already in phase and only amplitudes are modulated while \( k \)-vector is changed [Fig. 1(b), lower panel].

The expansion coefficients \( D_{p,p,mn} \) depend on shape of the nanoparticles, material parameters and symmetry of the lattice. Obviously, that the lattice symmetry should impose restrictions on \( D_{p,p,mn} \) and some coefficients should vanish due to the symmetry. To explore these selection rules, we employ theoretical-group approach.

III. SYMMETRY APPROACH

The group-theoretic approach is a powerful method which is widely used for analyzing the properties of periodic photonic system [30, 48–51]. In this section, we apply this method to reveal which of the coefficients \( D_{p,p,mn} \) are non-zero in accordance with the mode symmetry imposed by the symmetry of the periodic structure [52, 53] and to explain the formation of BIC. To make further analysis more illustrative we will provide it by the example of a square periodic array of dielectric spheres
operations the basis functions with different reducible representations labeled by \( \Gamma \) are already the basis functions of the translation group irreducible representation's symmetry group [54, 55]. While Bloch functions transformed by an irreducible representation of the structure's symmetry group \( \mathbf{g} \) see that additionally to \( \Gamma \)-BIC, TM modes have mainly the transverse electric (TE) and transverse magnetic modes \( \mathbf{T}M \). The \( z \)-component of the electric field \( E_z \) is shown by color in the inserts. Note that representations can be obtained by replacing for TE-modes \( A_2 \leftrightarrow B_1 \), \( u \leftrightarrow g \), and multipolar content can be obtained by replacing \( p_1 \leftrightarrow -p_1 \).

### Table I. Multipolar content and irreducible representations of TE-modes at the \( \Gamma \)-point and at \( \Gamma X \) and \( \Gamma M \) valleys.

| \( \Gamma \)-point | \( \mathbf{E}_x \)-field profile, representations | \( \mathbf{E}_z \)-field profile, representations |
|------------------|----------------------------------|----------------------------------|
| \( \Gamma \)-BIC | \( \mathbf{A}_6 \) | \( \mathbf{E}_x \), \( \mathbf{B}_4 \) |
| \( \Gamma X \) | \( \mathbf{N}_{112}, \mathbf{N}_{113}, \mathbf{N}_{114} \) | \( \mathbf{N}_{112}, \mathbf{N}_{113}, \mathbf{N}_{114} \) |
| \( \Gamma M \) | \( \mathbf{M}_{112}, \mathbf{M}_{113}, \mathbf{M}_{114} \) | \( \mathbf{M}_{112}, \mathbf{M}_{113}, \mathbf{M}_{114} \) |

### Table II. Multipolar content and irreducible representations of TM-modes. The \( z \)-component of the electric field \( E_z \) is shown by color in the inserts. Note that representations can be obtained by replacing for TE-modes \( A_2 \leftrightarrow B_1 \), \( u \leftrightarrow g \), and multipolar content can be obtained by replacing \( p_1 \leftrightarrow -p_1 \).

| \( \Gamma \)-point | \( \mathbf{E}_x \)-field profile, representations | \( \mathbf{E}_z \)-field profile, representations |
|------------------|----------------------------------|----------------------------------|
| \( \Gamma \)-BIC | \( \mathbf{A}_6 \) | \( \mathbf{E}_x \), \( \mathbf{B}_4 \) |
| \( \Gamma X \) | \( \mathbf{N}_{112}, \mathbf{N}_{113}, \mathbf{N}_{114} \) | \( \mathbf{N}_{112}, \mathbf{N}_{113}, \mathbf{N}_{114} \) |
| \( \Gamma M \) | \( \mathbf{M}_{112}, \mathbf{M}_{113}, \mathbf{M}_{114} \) | \( \mathbf{M}_{112}, \mathbf{M}_{113}, \mathbf{M}_{114} \) |

shown in the inset in Fig. 2(a). Nevertheless, it is necessary to highlight that further considerations remain true for any kind of structures with square lattice with the point group symmetry \( D_{4h} \).

Figure 2(a) shows the dispersion of eigenmodes along the \( \Gamma X \) direction for a square periodic array of dielectric spheres with permittivity \( \varepsilon_2 = 12 \) embedded in the air with permittivity \( \varepsilon_1 = 1 \). The dispersion is calculated numerically using COMSOL Multiphysics package. The radius of the spheres is \( a = 100 \) nm and the period of the array is \( d = 600 \) nm. By the analogy with a dielectric slab waveguide, the eigenmodes of the 2D array are split into transverse electric (TE) and transverse magnetic modes (TM), which have mainly the \( x \)-component of magnetic field \( H_x \) is shown by color in the inserts. The \( z \)-component of the magnetic field \( H_z \) transform through each other. They carry high-dimensional representations of the space group. We are interested in the multipolar content of the mode with particular \( k_b \) so we look at the point group of \( k_b \), i.e. the subgroup of the whole point group, which transforms the \( k_b \) into an equivalent.

### \( \Gamma \)-point. At the \( \Gamma \)-point, the group of \( k_b \) is the whole group \( D_{4h} \), \( k_b = 0 \) and it is not transformed. At \( \Gamma X \)-valleys the point group of \( k_b \) is \( C_{2v} \), which consists of \( \pi \)-rotation around the \( x \)- or \( y \)-axis and two plane reflections at \( z = 0 \) and at \( y = 0 \) or \( x = 0 \). These operations keep vector \( k_b \) invariant. Analogously, in the \( \Gamma M \)-valley the group is also \( C_{2v} \). Solutions with particular \( k_b \) are transformed by one of the \( k_b \)-group irreducible representations. Thus, since the solution is transformed as a basis function of some particular representation, the multipolar content is strictly limited. Namely, all the multipoles with non-zero contribution must be transformed by the similar irreducible representation of the \( k_b \)-group. For example, we consider the TE\(_1 \) mode of the square array, which is transformed by \( A_{2g} \) at the \( \Gamma \)-point. Under the transformations of \( D_{4h} \) group the only low-order multipoles transformed by \( A_{2g} \) are magnetic dipole \( \mathbf{M}_{-101} \), magnetic octupole \( \mathbf{M}_{-103} \), and electric hexadecapole \( \mathbf{N}_{-144} \). All of them are invariant under \( C_4 \) rotations, even under inversion and \( z = 0 \)-plane reflection and odd under other \( D_{4h} \) transformations. Higher-order multipoles which behave in the same way are also presented in the multipolar content of this mode.

Analogously, we classify all possible multipoles at the \( \Gamma \)-point in accordance with their symmetry and provide the tables with multipolar content of the modes (Tables I and II). Note, that TE\(_2 \) and TE\(_3 \) modes degenerate, and they transform through each other as two basis functions.
IV. MULTIPOLAR COMPOSITION OF THE EIGENMODES IN PERIODIC STRUCTURES

A. Periodic arrays of dielectric spheres

In order to understand how the interference of the multipole moments forms the BICs, we applied a method of multipole decomposition by expanding the eigenmodes fields inside the nanoparticles in terms of spherical harmonics [33, 34]. Figure 3 shows the numerical results for the multipole decomposition for TE1, TE4, and TM4 modes at the Γ-point and in a point of the ΓX-valley. At the high-symmetry Γ-point only a small fraction of all possible multipoles is presented, while after lowering the symmetry extra multipoles appear out of the Γ-point. Figure 4 shows the numerical results for the multipole decomposition for TM3 modes at the Γ-point, in a point of the ΓX-valley, and at the off-Γ BIC.

At-Γ-BIC. One can see, that for at-Γ TE1(A2g) BIC-mode magnetic dipole along the z-axis (M_{101}) is mainly contributed [Fig. 3(a)]. Its directivity pattern restricts radiation along the z-axis, and the radiation patterns of all remaining multipoles at the Γ-point are also zero along the z-axis. Other directions of radiation are forbidden due to the subdiffraction regime. Similarly, at-Γ TM3(A1u) BIC is formed by electric dipole along the z-axis (N_{101}) mostly, prohibiting the radiation in vertical direction itself [Fig. 4(a)]. The TE4 (B2g) and TM4 (B1u) modes’ lowest multipoles are the electric quadrupole N_{122} and the magnetic quadrupole M_{122} respectively. They have m = 2, which also prohibits the radiation [Figs. 3(c) and 3(e)]. In contrast to BICs, the radiative modes (E_g, E_u) are degenerate at the Γ point since they are transformed by the two-dimensional representations. From the symmetry-group approach, we know that TE_{2,3} and TM_{1,2} modes contain electric N_{±111} and magnetic M_{±111} spherical harmonics. The numerical multipole expansion shows that degenerated modes...
contain in-plane electric or magnetic dipole moments as the main contribution. These numerical results validate the symmetry-group approach for the system with square lattice, confirming that any symmetry-protected BIC is characterized by multipole moments with $m \neq 1$.

**Off-Γ BIC.** Away from the Γ-point other multipoles appear in decomposition [Figs. 3(b), 3(d), 3(f) and 4(b)] and BIC is destroyed turning into a resonance state. As mentioned earlier in the Section II, the accidental off-Γ BICs is formed due to either in- or anti-phase contributions of different multipoles. We obtain the same result for TM$_3$ mode with off-Γ BIC in the ΓX-valley [Fig. 4(c)]. This mode is transformed by $B_1$ representation and consist of the multipoles, which are odd under reflection in the $z = 0$ plane and $\pi$-rotation around $x$-axis and even under $y = 0$ reflection, e.g. $iN_{101}, N_{112}, iN_{103}, iN_{123}, M_{111}, iM_{112}, M_{113}, M_{133}$. They sum up into $TM$-polarized wave in the direction given by vector $k_1$ and cancel each other in the off-Γ point forming accidental BIC, shown in Fig. 2(b). In addition to all, it is well known, that the $z = 0$ plane reflection symmetry of the structure is required to obtain the off-Γ BIC [29]. Indeed, in lack of such symmetry, each mode would contain both odd and even multipoles under reflection in the $z = 0$ plane. To restrict the radiation both in the upper- and lower half-spaces, odd and even multipoles should be summed up into zero independently, while for the symmetric structure only one type of multipoles is presented for each mode, which makes it possible to achieve the BIC by tuning the structure parameters.

**B. Photonic crystal slab**

We extend our approach beyond the 2D array of spheres and apply it to the photonic crystal slab of the same symmetry. We consider a dielectric slab with a square array of cylindrical holes studied in [29]. Both at-Γ (symmetry-protected) and off-Γ (accidental) BICs appear in the lowest TM band referred to as TM$_h$. This mode has the field profile of the same symmetry as the TM$_4$ mode of the array of the spheres and is transformed...
by $B_{1u}$ representation.

The description of the far field defined by the Eq. (3) is still valid, but the coefficients $D_{p,p,mn}$ in general cannot be expressed analytically through $D_{p,p,mn}$ (see Appendix C). However, only the multipoles which are presented in the field inside the slab contribute into far field, $\tilde{D}_{p,p,mn} = 0$ if $D_{p,p,mn} = 0$. The multipolar content for the considered slab is the same as in the periodic array of spheres because the modes of the slab have the same symmetry as the modes of the array. The multipole decomposition of TM$_h$ mode [Fig. 5(a)] reveals that a magnetic quadrupole $M_{122}$ and electric octupole $N_{123}$ make the major contribution to the at-$\Gamma$ BIC, as well as to the TM$_4$ mode of the array of the spheres. However, the $B_{1u}$ mode of the photonic crystal slab is the lowest-energy TM mode while for the array of spheres it has the highest energy among modes under diffraction limit. Due to the variational principle [58], for the mode of such symmetry, the electric field is more concentrated inside the high-index material in case of photonic crystal slab, minimizing the energy of the mode. Although dispersion curves $\omega(k)$ of the modes TM$_4$ and TM$_h$ behave completely differently, multipole decomposition proves a common origin of them. At the $\Gamma$-point, we obtain contributions of multipoles only with $m = 2, 6, 10$, etc. for both modes, and none of these multipoles contribute in the far-field. At the $\Gamma\chi$-valley, the multipolar content of the TM$_4$ and TM$_h$ is similar [Figs. 3(e), 3(f), 5(a), 5(b)]. However, for the TM$_h$ it is possible to obtain an accidental off-$\Gamma$ BIC in the $\Gamma\chi$-valley [Fig. 5(c)]. Away from the $\Gamma$-point, multipole contributions change smoothly keeping the multipolar content invariable, and at a particular wave vector $k_x$ multipoles interfere destructively forming the accidental BIC.

V. SUMMARY AND OUTLOOK

Importantly, our approach based on the multipole decomposition analysis of individual meta-atoms not only explains clearly and in simple physical terms the origin of both symmetry protected and accidental bound states in the continuum, but it has also a prediction power and may be employed for both prediction and engineering different types of BICs. As an example, we consider a metasurface consisting of meta-atoms packed in a subwavelength 2D lattice, which are polarized purely as octupoles, for example, $N_{103}$ (see Fig. 6). Each octupole of this type has a nodal cone and, therefore, we can expect that in a periodic subwavelength array of such meta-atoms, BICs form a line in the reciprocal space. However, to observe this phenomenon, the effective polarizability of the unit cell accounting for the interaction between all meta-atoms should not depend on the Bloch wavenumber or have very weak dependence. In other words, the line of BIC could be observed in metasurfaces with suppressed spatial dispersion that is still a challenging problem. It is interesting that such a kind of BIC will be observed for the same directions independently on the lattice symmetry of the metasurface. Thus, the multipole origin of BIC makes a new query for metasurfaces with a suppressed spatial dispersion.

In summary, we have demonstrated that symmetry-protected bound states in the continuum in dielectric metasurfaces at the frequencies below the diffraction limit are associated with the multipole moments of the elementary meta-atoms which do not radiate in the transverse direction. For any type of metasurfaces, the symmetry-protected bound states in the continuum can be observed only if there exist no multipoles with the azimuthal index $m = 1$ in the multipole decomposition. The symmetry approach allows to determine which multipolar content the lattice eigenmodes have, and it can be analogously applied to the structures with different symmetries, for example, hexagonal lattices or arrays of nanoparticles of an arbitrary shape and in-plane broken symmetry. Similarly, we have revealed that the accidental bound state in the continuum corresponding to an off-$\Gamma$ point in the reciprocal space are formed due to destructive interference of the multipole fields in the far-zone. We have provided the general tools for the analysis of bound states in the continuum based on the irreducible representation of the appropriate photonic band. We believe that our results will provide a new way for designing high-quality resonant photonic systems based on the physics of bound states in the continuum.

ACKNOWLEDGMENTS

The authors acknowledge useful discussions with I.D. Avdeev. Y.K. acknowledges a support from the Strategic Fund of the Australian National University. Z. S. acknowledges support from the Foundation for the Advancement of Theoretical Physics and Mathematics "BASIS" (Russia).

Z.S. and K.F. contributed equally to this work.
S. Romano, A. Lamberti, M. Masullo, E. Penzo, J. M. Foley, S. M. Young, and J. D. Phillips, Symmetry-

J. M. Foley and J. D. Phillips, Normal incidence narrow-band transmission filtering in a dielectric grating, Phys. Rev. B 61, 2090 (2000).

E. N. Bulgakov and A. F. Sadreev, Bound states in the continuum in photonic waveguides inspired by defects, Phys. Rev. B 78, 075105 (2008).

D. C. Marinica, A. G. Borisov, and S. V. Shabanov, Bound States in the Continuum in Photonics, Phys. Rev. Lett. 100, 183902 (2008).

F. Dreisow, A. Szameit, M. Heinrich, R. Keil, S. Nolte, A. Tümmermann, and S. Longhi, Adiabatic transfer of light via a continuum in optical waveguides., Opt. Lett. 34, 2405 (2009).

C. M. Gentry and M. A. Popović, Dark state lasers, Opt. Lett. 39, 4136 (2014).

S. T. Ha, Y. H. Fu, N. K. Emani, Z. Pan, R. M. Bakker, R. Paniagua-Dominguez, and A. I. Kuznetsov, Directional lasing in resonant semiconductor nanoantenna arrays, Nat. Nanotechnol. 13, 1042 (2018).

K. Koshelev, A. Bogdanov, and Y. Kivshar, Meta-optics guided resonances robust to out-of-plane scattering, arXiv preprint arXiv:1812.00892 (2018).

W. Chen, Y. Chen, and W. Liu, Singularities and Poincaré indexes of electromagnetic multipole, arXiv preprint arXiv:1901.04159 (2019).

D. R. Abujetas, A. Barreda, F. Moreno, J. J. Saenz, A. Litman, J.-M. Gérard, and J. A. Sanchez-Gil, Brewster quasi bound states in the continuum in all-dielectric metasurfaces from single magnetic-dipole resonance meta-atoms, arXiv preprint arXiv:1902.07148 (2019).

Y. V. Kartashov, C. Milián, V. V. Konotop, and L. Torner, Bound states in the continuum in a two-dimensional PT-symmetric system, Opt. Lett. 43, 575 (2018).

S. Romano, G. Zito, S. Managò, G. Calafiore, E. Penzo, S. Cabrini, A. C. De Luca, and V. Mocella, Surface-enhanced raman and fluorescence spectroscopy with an all-dielectric metasurface, J. Phys. Chem. C 122, 19738 (2018).

E. Bulgakov and A. Sadreev, Trapping of light with angular orbital momentum above the light cone, Advanced Electromagnetics 6, 1 (2017).

C. Wei Hsu, B. Zhen, S.-L. Chua, S. G. Johnson, J. D. Joannopoulos, and M. Soljačić, Bloch surface eigenstates within the radiation continuum, Light Sci. Appl. 2, e84 (2013).

B. Zhen, C. W. Hsu, L. Lu, A. D. Stone, and M. Soljačić, Topological Nature of Optical Bound States in the Continuum, Phys. Rev. Lett. 113, 257401 (2014).

C. W. Hsu, B. Zhen, J. Lee, S.-L. Chua, S. G. Johnson, J. D. Joannopoulos, and M. Soljačić, Observation of trapped light within the radiation continuum, Nature 499, 188 (2013).

P. Yu, A. S. Kuprianov, V. Dmitriev, and V. R. Tuz, All-dielectric metasurfaces with trapped modes: group-theoretical description, arXiv:1812.10817 [physics.optics] (2018).

L. Ni, Z. Wang, C. Peng, and Z. Li, Tunable optical bound states in the continuum beyond in-plane symmetry protection, Phys. Rev. B 94, 245148 (2016).

H. Friedrich and D. Wintgen, Interfering resonances and bound states in the continuum, Phys. Rev. A 32, 3231 (1985).

J. Jackson, Classical electrodynamics (Wiley, 1999).

P. Grahn, A. Shevchenko, and M. Kaivola, Electromagnetic multipole theory for optical nanomaterials, New J. Phys. 14, 093033 (2012).

S. S. Kruk, R. Camacho-Morales, L. Xu, M. Rahmani, D. Smirnova, L. Wang, H. H. Tan, C. Jagadish, D. N. Neshev, and Y. S. Kivshar, Nonlinear optical magnetism revealed by second-harmonic generation in nanoantenn-
9

[36] A. B. Evlyukhin, C. Reinhardt, A. Seidel, B. S. Luk’yanchuk, and B. N. Chichkov, Optical response features of Si-nanoparticle arrays, Phys. Rev. B 82, 045404 (2010).

[37] A. I. Kuznetsov, A. E. Miroshnichenko, M. L. Brongersma, Y. S. Kivshar, and B. Luk’yanchuk, Optically resonant dielectric nanostructures, Science 354, aug2472 (2016).

[38] M. Panmai, J. Xiang, Z. Sun, Y. Peng, H. Liu, H. Liu, Q. Dai, S. Tie, and S. Lan, All-silicon-based nanoantennas for wavelength and polarization demultiplexing, Opt. Express 26, 12344 (2018).

[39] K. Baryshnikova, D. Filonov, C. Simovski, A. Evlyukhin, A. Kadochkin, E. Nenasheva, P. Ginzburg, and A. S. Shalin, Giant magnetoelectric field separation via anapole-type states in high-index dielectric structures, Phys. Rev. B 98, 165419 (2018).

[40] P. C. Wu, C. Y. Liao, V. Savinov, T. L. Chung, W. Chen, Y.-W. Huang, P. R. Wu, Y.-H. Chen, A.-Q. Liu, N. Zheludev, and D. P. Tsai, Optical anapole metamaterial, ACS Nano 12, 1920 (2018).

[41] W. Hsu, Novel Trapping and Scattering of Light in Resonant Nanophotonic Structures, Ph.D. thesis (2015).

[42] A. V. Poshakinskiy and A. N. Poddubny, Optomechanical kerker effect, Phys. Rev. X 9, 011008 (2019).

[43] H. K. Shamkhi, K. V. Baryshnikova, A. Sayanskiy, P. Kapitanova, P. D. Terekhov, A. Karabchevsky, A. B. Evlyukhin, P. Belov, Y. Kivshar, and A. S. Shalin, Transverse scattering with the generalised kerker effect in high-index nanoparticles, arXiv preprint arXiv:1808.10708 (2018).

[44] W. Liu and Y. S. Kivshar, Generalized kerker effects in nanophotonics and meta-optics (invited), Opt. Express 26, 13085 (2018).

[45] C. F. Bohren and D. R. Huffman, Absorption and scattering of light by small particles, (Wiley, 1983) pp. xiv, 530 p.

[46] K. Frizyuk, Second harmonic generation in dielectric nanoparticles with different symmetries, arXiv preprint arXiv:1812.02988 (2018).

[47] J. A. Stratton, Electromagnetic Theory (2007) pp. 392–423.

[48] W. Hergert and M. Dane, Group theoretical investigations of photonic band structures, Phys. Status Solidi (a) 197, 620 (2003).

[49] K. Ohtaka and Y. Tanabe, Photonic band using vector spherical waves. I. various properties of bich electromagnetic fields and heavy photons, J. Phys. Soc. Jpn. 65, 2265 (1996).

[50] K. Ohtaka and Y. Tanabe, Photonic bands using vector spherical waves. III. group-theoretical treatment, J. Phys. Soc. Jpn. 65, 2670 (1996).

[51] K. Sakoda, Optical properties of photonic crystals (Springer series in optical sciences, vol. 80), (2001).

[52] S. Hayami, M. Yatsushiro, Y. Yanagi, and H. Kusunose, Classification of atomic-scale multipoles under crystallographic point groups and application to linear response tensors, Phys. Rev. B 98, 165110 (2018).

[53] A. Gelessus, W. Thiel, and W. Weber, Multipoles and symmetry, J. Chem. Educ. 72, 505 (1995).

[54] V. M. Agranovich and V. Ginzburg, Crystal optics with spatial dispersion, and excitons, Vol. 42 (Springer Science and Business Media, 2013).
Appendix A: Basic definitions

Vector spherical harmonics are defined as [45]

\[
\mathbf{M}_{m,n}^{(1)} = \nabla \times (r\psi_{m,n}), \quad (A1)
\]
\[
\mathbf{N}_{m,n}^{(1)} = \frac{\nabla \times \mathbf{M}_{m,n}^{(1)}}{k}, \quad (A2)
\]

where

\[
\psi_{1mn} = \cos m\varphi P_n^m(\cos \theta) z_n(kr),
\]
\[
\psi_{-1mn} = \sin m\varphi P_n^m(\cos \theta) z_n(kr)
\]

\(z_n(kr)\) can be replaced by spherical Bessel function of any kind, and \(P_n^m(\cos \theta)\) are associated Legendre polynomials.

Vacuum dyadic Green’s function expansion in terms of vector spherical harmonics [59, 60]:

\[
\hat{G}_0(r,r') = \frac{ik_1}{4\pi} \sum_{n=1}^{\infty} \sum_{\pm=1} \sum_{m=0}^{n} (2 - \delta_0) \frac{2n+1}{n(n+1)(n+m)!} \left( \mathbf{M}_{p,pmn}^{(3)}(k_1,r) \otimes \mathbf{M}_{p,pmn}^{(1)}(k_1,r') + \mathbf{N}_{p,pmn}^{(3)}(k_1,r) \otimes \mathbf{N}_{p,pmn}^{(1)}(k_1,r') \right), \quad r > r'
\]

where superscripts (1) and (3) appear, when we replace \(z_n(\rho)\) by spherical Bessel functions, and the spherical Hankel functions of the first kind, respectively, \(\delta_0 = 1\) when \(m = 0\), and \(\delta_0 = 0\) when \(m \neq 0\).

Spherical vectors \(\mathbf{Y}_{p,pmn}\) denote two types of functions, \(\mathbf{X}_{p,pmn}\) and \(\mathbf{Z}_{p,pmn}\), defined as [61]

\[
\mathbf{X}_{-p,pmn} \left( \frac{k}{k} \right) = \nabla \times \left( k\mathbf{Y}_{p,pmn} \left( \frac{k}{k} \right) \right)
\]
\[
\mathbf{Z}_{p,pmn} \left( \frac{k}{k} \right) = \frac{k}{k} \times \mathbf{X}_{-p,pmn} \left( \frac{k}{k} \right)
\]

where

\[
Y_{1mn} = \cos m\varphi P_n^m(\cos \theta)
\]
\[
Y_{-1mn} = \sin m\varphi P_n^m(\cos \theta)
\]

\(p_i = (-1)^{n+1}\) for \(\mathbf{X}\), and \(p_i = (-1)^n\) for \(\mathbf{Z}\). Note that the transformation behavior is similar for \(\mathbf{W}\) and \(\mathbf{Y}\), \(\mathbf{X}\) and \(\mathbf{M}\), \(\mathbf{Z}\) and \(\mathbf{N}\), \(\psi\) and \(Y\), respectively.

Appendix B: Lattice sums of the spherical harmonics

We assume that multipolar content of the mode is already known, and coefficients in the formula (1) are given. With help of vacuum dyadic Green’s function \(\hat{G}_0\), we express the field outside the array

\[
\mathbf{E}(r) = \frac{k_1^2}{4\pi} \int d^2r'' \Delta \varepsilon(r'') \hat{G}_0(r, r'') \mathbf{E}^{in}(r'') = \frac{k_1^2}{4\pi} (\varepsilon_2 - \varepsilon_1) \sum_j \int d^3r' \hat{G}_0(r, r_j + r') \mathbf{E}^{in}(r_j + r')
\]

where \(k_1 = \sqrt{\varepsilon_2 / \varepsilon_1}\) is vacuum wavevector, \(V\) is the single nanoparticle’s volume.

Green’s function can be also expressed in terms of vector spherical harmonics (see Appendix A). Using the property \(\hat{G}_0(r, r_j + r', \omega) = \hat{G}_0(r - r_j, r', \omega)\), and substituting (1) into (B1), we obtain
\[ E(\mathbf{r}) = E_0 \sum_{j} \frac{ik^3(\varepsilon_2 - \varepsilon_1)}{(4\pi)^2} \sum_{p',n,m} (2 - \delta_0) \frac{2n+1}{n(n+1)} \frac{(n-m)!}{(n+m)!} D_{p',p',n,m'} \mathbf{W}_{p',p',n,m'}^{(3)}(k_1, \mathbf{r} - \mathbf{r}_j). \]

where \[ \delta \] is the Kronecker delta. It is proportional to spherical Hankel functions \[ \delta \] is replaced by spherical Hankel functions \[ \text{inside the sphere}. \] If the fields created by each unit cell are already known, we can also start the considerations from the volume integral \[ \hat{D} \] is connected with

\[ \mathbf{E}(\mathbf{r}) = E_0 \sum_{p',n,m} \hat{D}_{p',p',n,m} \mathbf{W}_{p',p',n,m}^{(3)}(k_1, \mathbf{r} - \mathbf{r}_j). \]

Note, that coefficient \( \hat{D}_{p',p',n,m} \) is non-zero only if the harmonic with such numbers is presented in the field expansion inside the sphere. If the fields created by each unit cell are already known, we can also start the considerations from this formula.

To obtain formula \( (2) \) we exploit the Weyl identity for VSH expansion through the plane waves in case when \( \delta \) is replaced by spherical Hankel functions \[ \text{inside the sphere}. \] If the fields created by each unit cell are already known, we can also start the considerations from this formula.

\[ \mathbf{E}(\mathbf{r}) = E_0 \sum_{p',n,m} \hat{D}_{p',p',n,m} \mathbf{W}_{p',p',n,m}^{(3)}(k_1, \mathbf{r} - \mathbf{r}_j). \]

Appendix C: Relation between the coefficients \( D \) and \( \hat{D} \)

The coefficients \( D \) in \( (2) \) and \( \hat{D} \) \( (3) \) are connected by the formula:

\[ \hat{D}_{p',p',n,m} = \frac{ik^3(\varepsilon_2 - \varepsilon_1)}{(4\pi)^2} (2 - \delta_0) \frac{2n+1}{n(n+1)} \frac{(n-m)!}{(n+m)!} D_{p',p',n,m'} \int d^3\mathbf{r}' \delta(\mathbf{r}' - \mathbf{r}) |\mathbf{W}_{p',p',n,m'}^{(1)}(k_1, \mathbf{r}') \mathbf{W}_{p',p',n,m'}^{(3)}(k_2, \mathbf{r}')| \]

(C1)
This formula describes both array of nanoparticles, and any photonic crystal slab, but in case of the array of spheres, the integral can be easily taken analytically.

**Remark** Here we give the dyadic Green’s function $\hat{G}_0(\mathbf{r}, \mathbf{r}')$ only for the case when $r > r'$. In case of photonic crystal slab or non-spherical particles, we also need the part of Green’s function when $r' < r$ [60] to obtain the near-field. This will alter the intermediate calculations, since we have to compute the lattice sum for VSHs with spherical bessel functions. Nevertheless, the answer will have the same form.

We apply the orthogonality properties of vector spherical harmonics [47] [p.418], and consider integrals of magnetic and electric harmonics separately. Implementing the angular integration, we reduce the integral to the integral of $r$-dependent Bessel functions products, which also can be computed analytically. For magnetic harmonics we have

$$\hat{D}^M_{p_1 p_2 m_1 m_2} = i D^M_{p_1 p_2 m_1 m_2} a^2 \varepsilon_1 [k_1^2 j_{n-1}(k_1 a) j_n(k_2 a) - k_1 k_2 j_{n-1}(k_2 a) j_n(k_1 a)]$$ \hspace{1cm} (C2)

where $a$ is nanoparticle radius, and for electric

$$\hat{D}^N_{p_1 p_2 m_1 m_2} = i D^N_{p_1 p_2 m_1 m_2} a^2 \varepsilon_1 \left( \frac{n+1}{2n+1} [k_1^2 j_{n-2}(k_1 a) j_{n-1}(k_2 a) - k_1 k_2 j_{n-2}(k_2 a) j_{n-1}(k_1 a)] + \right.$$

$$\left. + \frac{n}{2n+1} [k_1^2 j_n(k_1 a) j_{n+1}(k_2 a) - k_1 k_2 j_n(k_2 a) j_{n+1}(k_1 a)] \right)$$ \hspace{1cm} (C3)

Note that this expression turns to zero at some frequencies, so we can have zero $\hat{D}$ when $D$ is non-zero. This refers to the anapoles of the spherical nanoparticles. The frequency where the anapole appears is the same as for single isolated nanoparticle.

If we have other type of surface, for example, photonic crystal slab with holes, or array of the cylinders, the orthogonality property can’t be applied and the integral $\int d^3r' \Delta \varepsilon \left[ W^{(1)}_{p_1 p_2 m_1}(k_1, \mathbf{r}') \cdot W^{(1)}_{p_2 p_1 m_2}(k_2, \mathbf{r}') \right]$ will mix some harmonics. However, all the harmonics, which admix, are already presented in the expansion of the field inside the cell. This will just alter the coefficients before the outgoing multipoles, but not the multipolar content.