Topological Bound States in the Continuum in Arrays of Dielectric Spheres

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We consider Bloch bound states in the radiation continuum in periodic arrays of dielectric spheres. It is demonstrated that the bound states are associated with phase singularities of the quasimode coupling strength. That makes the bound states topologically protected and, therefore, robust against any variation of parameters preserving the periodicity and rotational symmetry about the array axis. It is shown that under variation of parameters the bound states can only be destroyed by either annihilation of the topological charge or by migration to the sector of the parametric space where the second radiation channel is open.

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Because of numerous applications [1] the ability to confine light at the nanoscale has become a topic of great interest in modern science. It is known that as long as outgoing waves of the same symmetry are allowed in the surrounding medium an optical state would lose its energy to the environment. Consequently, the major challenge in engineering optical bound states is to suppress the radiation channels. The most trivial solution is to employ the guided modes below the line of light which are protected by the total internal reflection [2]. Another opportunity is to cloak the light guiding structure with Bragg mirrors that block radiative losses by the photonic band gap [3]. Both methods virtually exploit the same idea of providing only evanescent contribution in the far field zone. It is far less trivial though to engineer a bound state when outgoing waves are allowed within the given range of parameters, say, above the line of light. The key idea is to use periodic structures which in the far zone support an infinite number of diffraction channels only one of them open at a selected frequency. It turns out then, quite unexpectedly, that at a specific set of the control parameters the periodic structure can support a source-free localized solution *accidentally* decoupled from the open channel being, of course, smoothly extended to the far zone over the evanescent ones [4]. Such solutions with discrete eigenfrequency embedded in the continuous spectrum of the scattering states are know as bound states in the continuum (BSCs) [5]. The idea of BSC dates back to the 1929 paper by von Neumann and Wigner [6]. Since then the BSCs have been addressed in various atomic, solid state, optical, and acoustic systems (see Ref. [5] and references therein).

So far most theoretically proposed and all experimentally observed optical BSCs are realized in extended structures because BSCs are forbidden in compact systems [5,7] with an exception of structures coated with zero-epsilon metamaterials [8]. Thus, as soon as a pure all-dielectric system is considered, one needs a structure infinitely extended at least in one dimension while confined in the other two. To the best of our knowledge the only all-dielectric two-dimensionally confined BSC-supporting structure known in the literature, albeit theoretically, is a linear periodic array of high-index dielectric spheres [9]. It is worth noticing that though two-dimensionally confined optical BSCs have been achieved experimentally the supporting structures were extended at least in two dimensions [10]. In regard to the symmetry it is self-evident that any solution symmetrically mismatched with the outgoing wave must be a BSC. Such symmetry protected BSCs [11] are already seen as an important tool in photonics with applications to normal incidence narrow-band filters [12] and light enhancement [13]. More interesting is that periodic structures allow for a different class of BSCs in the form of traveling or Bloch waves that are not symmetrically mismatched with the outgoing solutions [4,14]. In 2014, Bo Zhen *et al.* [15] demonstrated that such BSCs in dielectric slabs are vortex centers in the polarization directions of far-field radiation. They carry conserved and quantized topological charges, defined by the winding number of the polarization vectors, which ensure their robust existence and govern their generation, evolution, and annihilation. It is been conjectured that all BSCs in all-dielectric periodic structure fall within two generic types, namely, symmetry protected and topologically protected ones [5]. Here we examine the Bloch BSCs in arrays of dielectric subwavelength spheres to demonstrate that they are associated with topological singularity of the quasi-mode coupling strength.

The system under consideration is an array of dielectric spheres with permittivity ϵ in air shown in Fig 1. The extensive numerical simulations have demonstrated that in that system there exists a single TE (but not TM) Bloch BSC, where TE, TM stand for pure transverse electric and transverse magnetic modes [9], correspondingly. The computational procedure was based on the numerically efficient method developed by Linton, Zalipaev, and Thompson [16]. According to Ref. [16] the magnetic

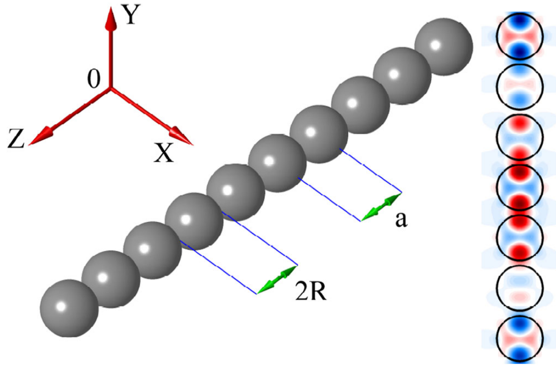

FIG. 1. Periodic array of dielectric spheres of radius R with period a. TE Bloch BSC exists at $k_z a = 0.859$, $k_0 a = 3.571$, $R = 0.450a$, $\epsilon = 12$ with k_z as the Bloch vector, and k_0 the vacuum wave number. The BSC magnetic field $\Re\{H_z\}$ in the $y0z$ plane is shown on the right.

vector $\mathbf{H}$ could be found as a series over spherical vector harmonics $\mathbf{N}_l^m(\mathbf{r}), \mathbf{M}_l^m(\mathbf{r})$

$$\mathbf{H}(\mathbf{r}) = -i\sqrt{\epsilon}\sum_{j=-\infty}^{\infty} e^{iajk_z}\sum_{l=m^*}^{\infty}[a_l^m\mathbf{N}_l^m(\mathbf{r}_j) + b_l^m\mathbf{M}_l^m(\mathbf{r}_j)], \quad (1)$$

where j is the number of the particle in the array, $\mathbf{r}_j$ the coordinate vector in the jth sphere reference frame, m the azimuthal number, and $m^* = \max(1, m)$. In what follows we only consider the case of zero orbital angular momentum (OAM) $m = 0$. Although originally used for the guided modes below the line of light [16] the method is shown to converge rapidly [17] above the line of light with the number of multipoles in the expansion Eq. (1). When the scattering problem is addressed one can demonstrate after some algebra [9] that for TE modes $b_l^0 = 0$, while the coefficient a_l^0 can be found by solving a set of linear equations,

$$\hat{L}\mathbf{p} = \mathbf{q}, \quad (2)$$

where $\mathbf{p}$ is the vector of coefficients a_l^0, $\mathbf{q}$ is the vector containing the expansion coefficients of the impinging TE wave over spherical harmonics, and $\hat{L}$ the interaction matrix. In our case the impinging TE solutions in the far-field zone can be described by the only nonzero component of the magnetic vector H_z [9],

$$H_z(r, \phi, z) = J_0(\chi_n r)e^{ik_z z}, \quad (3)$$

with

$$\chi_n^2 = k_0^2 - (k_z + 2\pi n/a)^2, \qquad n = 0, \pm 1, \pm 2, \ldots, \quad (4)$$

where r, z are the cylindrical coordinates, $J_0(\chi_n r)$ is the Bessel function, k_0 is the vacuum wave number, and k_z is the Bloch vector. In what follows we will stay above the light line $k_0 = k_z$ in the range $k_z a < k_0 a < \pi - k_z a$, which, according to Eq. (4), means that only one channel $n = 0$ is open. Henceforth, we will use $\mathbf{q}_0$ for the expansion coefficients of this channel.

At this point we return to Ref. [15] where the Bloch BSCs in dielectric slabs were associated with singularities of the polarization directions in far field radiation. In our case the total electromagnetic field with zero OAM is split into pure (totally decoupled) TE and TM solutions [9] and the far-field pattern is given by a single radiation channel (3) with a definite polarization to render the polarization approach inapplicable. In other words, as the parameters R, a, and ϵ are detuned from the BSC the TE solution remains decoupled from the TM channel with the polarization direction remaining the same. Here to construct a topological invariant we analyze the formal solution of Eq. (2). The interaction matrix $\hat{L}$ in Eq. (2) contains multipole Mie coefficients as well as the infinite lattice sums describing multiple scattering events between the spheres. We refer the reader to Refs. [9,16] for the exact structure of $\hat{L}$. Importantly, according to Ref. [16] $\hat{L}$ has the following property:

$$L_{l,l'} = (-1)^{l+l'}L_{l',l}, \quad (5)$$

and, hence, is not Hermitian. For further analysis we will use the quasimodal expansion [18] based on the biorthogonal basis of left $\mathbf{y}_s$ and right $\mathbf{x}_s$ eigenvectors

$$\hat{L}\mathbf{x}_s = \lambda_s\mathbf{x}_s, \quad \hat{L}^\dagger\mathbf{y}_s = \lambda_s^*\mathbf{y}_s, \quad \mathbf{y}_s^\dagger\mathbf{x}_{s'} = \mathbf{x}_s^\dagger\mathbf{y}_{s'} = \delta_{s,s'}. \quad (6)$$

Then, the inverse of $\hat{L}$ is then given by

$$\hat{L}^{-1} = \sum_s \frac{1}{\lambda_s}\mathbf{x}_s\mathbf{y}_s^\dagger. \quad (7)$$

It should be noticed that $\hat{L}$, and, thus, λ_s, $\mathbf{x}_s$, $\mathbf{y}_s$ are dependent on both k_z and k_0 [9]. By using Eq. (5) one can show that

$$\{\mathbf{y}_s\}_l = (-1)^l\{\mathbf{x}_s^*\}_l. \quad (8)$$

Notice that Eq. (8) along with the normalization condition in Eq. (6) simultaneously allow only freedom in choosing prefactor ± 1 in front of $\mathbf{x}_s$. Further on we assume that the signs of $\mathbf{x}_s$ are consistently defined in the space of k_z, k_0. Applying Eq. (7) we can write the solution of the scattering problem (2) in the following form:

$$\mathbf{p} = \sum_s \frac{\mathcal{W}_s}{\lambda_s}\mathbf{x}_s, \mathcal{W}_s = \mathbf{y}_s^\dagger\mathbf{q}_0. \quad (9)$$

Finally, by using $\{\mathbf{q}\}_l = (-1)^l\{\mathbf{q}^*\}_l$ [9] together with Eq. (8) one can write

$$\mathcal{W}_s = \mathbf{q}_0^\dagger \mathbf{x}_\mathbf{s}, \tag{10}$$

which can be interpreted as the expansion of quasimode $\mathbf{x}_\mathbf{s}$ over the impinging wave. Further on $\mathcal{W}_s$ will be refereed to as the quasimode coupling strength.

In the BSC point a source-free solution of Eq. (2) must exist even without the array being illuminated from the far zone to yield a simple condition for a BSC

$$\det[\hat{L}(k_0, k_z)] = 0. \tag{11}$$

The above condition means that in the BSC point there is an eigenvector $\mathbf{x}_0$ with zero eigenvalue

$$\hat{L}^\dagger \mathbf{x}_0 = 0, \tag{12}$$

obviously corresponding to the BSC mode shape. On the other hand, by transforming Eq. (2) to the biorthogonal basis [19] in which the interaction matrix is diagonal $\hat{L} = \mathrm{diag}[\lambda_1, \lambda_2, \ldots]$ one finds in the BSC point

$$\mathcal{W}_0 = \mathbf{q}_0^\dagger \mathbf{x}_0 = 0; \tag{13}$$

i.e., the BSC is orthogonal to the incident wave $\mathbf{q}_0$.

The quasimode coupling strength is in general complex valued to be written as

$$\mathcal{W}_0(k_0, k_z) = f(k_0, k_z) + i g(k_0, k_z), \tag{14}$$

where $f(k_0, k_z), g(k_0, k_z)$ are real valued functions. In Fig. 2 we plot the phase of $\mathcal{W}_0(k_0, k_z)$,

$$\theta = \arg(\mathcal{W}_0), \tag{15}$$

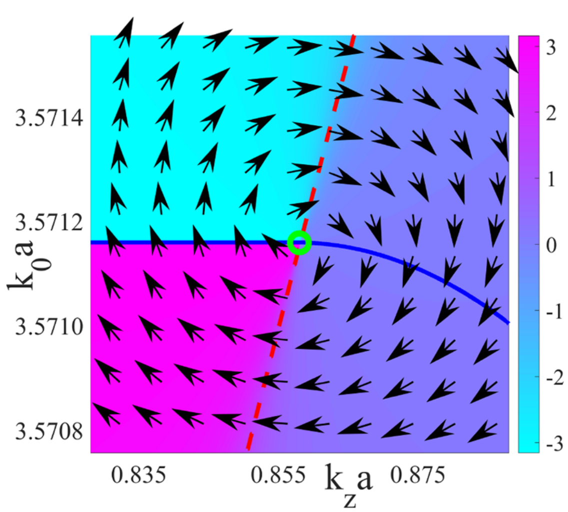

FIG. 2. Phase θ of the coupling strength $\mathcal{W}_0$ at the BSC from Fig. 1 shown by the green circle. Nodal lines $f(k_0, k_z) = 0$ and $g(k_0, k_z) = 0$ are shown by the dashed red and solid blue lines, correspondingly. The arrows are aligned with the direction of $\mathbf{j}$ Eq. (16).

in the parametric vicinity of the Bloch BSC from Fig. 1. One can see from Fig. 2 that the BSC sits on the intersection of the nodal lines $f(k_0, k_z) = 0$ and $g(k_0, k_z) = 0$, thus being a singular point of phase θ. Finally, by introducing vector

$$\mathbf{j} = \nabla\theta \tag{16}$$

one can demonstrate that the BSC is the center of a vortex in space of k_0, k_z.

The above picture is generic for phase singularities in complex fields nicely described by Dennis [20]. What is important, the singularity associated with a topological charge is specified by the winding number

$$q = \mathrm{sgn}\left(\frac{\partial f}{\partial k_0}\frac{\partial g}{\partial k_z} - \frac{\partial g}{\partial k_0}\frac{\partial f}{\partial k_z}\right), \tag{17}$$

which prescribes either clockwise $q = 1$ or counterclockwise $q = -1$ circulation of $\mathbf{j}$ around the singular point [20]. The freedom in choosing the sign of $\mathbf{x}_\mathbf{s}$ affects neither the winding number Eq. (17) nor the position of the nodal point since it only flips the sign of both $f(k_0, k_z)$ and $g(k_0, k_z)$ simultaneously. From the mirror symmetry with respect to $z \to -z$ it immediately follows that there exists a complex conjugate Bloch BSC propagating in the opposite direction with vector $-k_z$. By changing the sign of $g(k_0, k_z)$ in Eq. (17) one finds that this BSC has a winding number opposite to that of its complex conjugate. This observation gives us a cue to the BSC evolution scenario under variation of the control parameters with subsequent annihilation of the topological charge. The generic picture is the following [20]. First, the topological charge is robust against small variation of the parameters such as a, R, and ϵ, for the nodal lines only slightly change their configuration in space k_0, k_z. As the parameters are changed further the pair of singularities with the opposite charge approach the annihilation point in which the nodal lines are tangent to each other. Finally, after the annihilation has occurred the nodal lines depart from one another. The above scenario is illustrated in Fig. 3(a).

As it follows from the mirror symmetry $z \to -z$ the annihilation point must have $k_z = 0$. In Figs. 3(b), 3(c) we illustrate the above speculation with numerical data. One can see from Fig. 3(b) that two singularities with opposite winding number sitting on the intersection of the nodal lines approach each other in space k_0, k_z while Fig. 3(c) shows a phase discontinuity that can only be relocated but not removed by a phase shift $\theta \to \theta + \mathrm{const}$. To check the robustness of the Bloch BSC we numerically traced its evolution under variation of both R and ϵ starting from the BSC in Fig. 1. The results are shown in Fig. 4 where one can see that with the increase of both R and ϵ the position of the BSC shifts towards the annihilation point $k_z = 0$, where the BSC disappears through annihilation with its complex

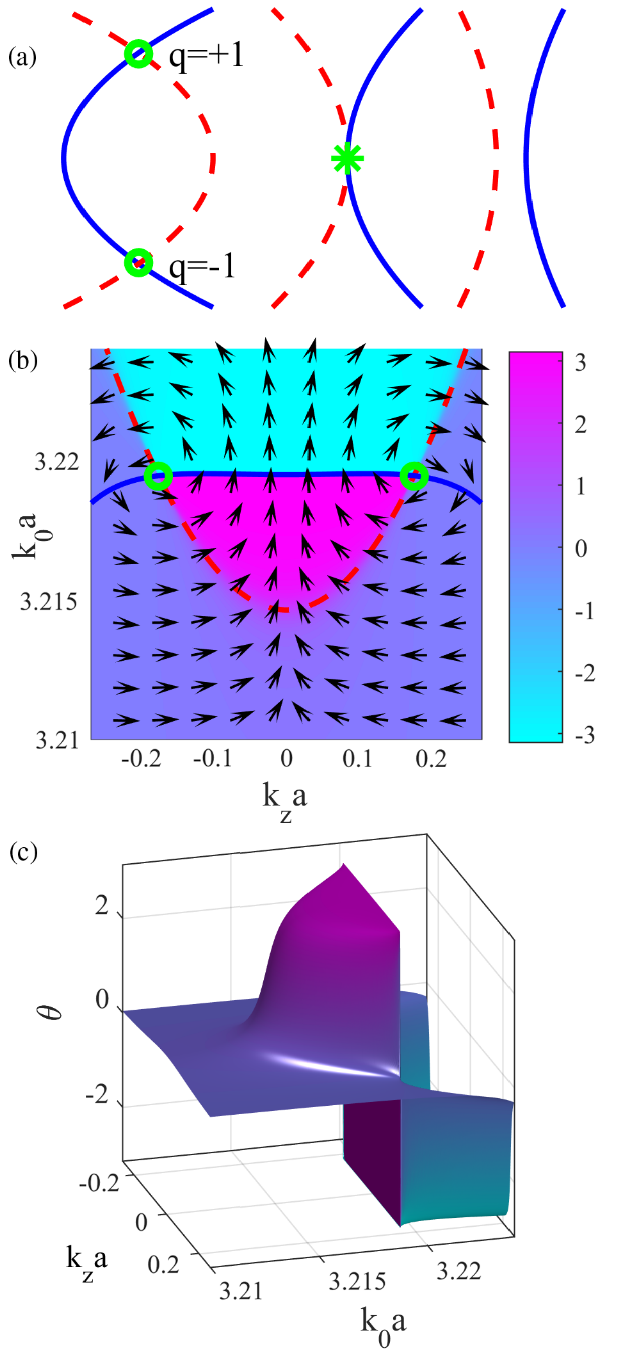

FIG. 3. Phase singularities of $\mathcal{W}_0$. (a) Generic of the scenario for the evolution towards the annihilation of the topological charge. The annihilation point is shown by the green star. (b) The same as Fig. 2 but for $R = 0.487a$. (c) Three-dimensional plot with the same data as in (b).

conjugate. On the other hand, with the decrease of R and ϵ the BSC migrates to larger values of k_z, k_0 and eventually arrives at the line $k_0a = 2\pi - k_za$ to be destroyed by leakage into the second radiation channel.

Finally, let us consider the annihilation in more detail. To do this we numerically found the resonant eigenfrequency $\omega = \Omega + i\Gamma$, where Ω is the resonance position and Γ the

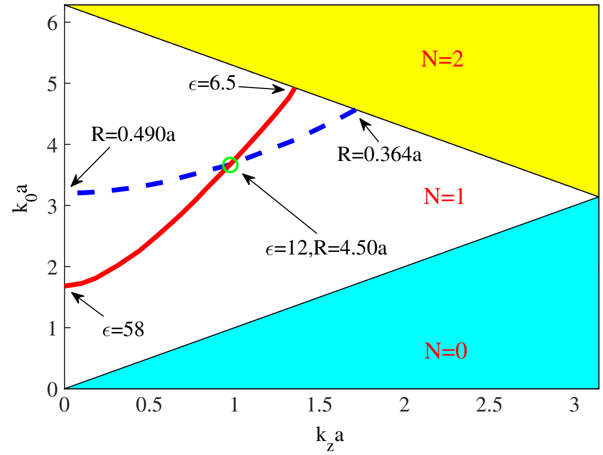

FIG. 4. Evolution of topologically protected BSC from Fig. 1 under variation of R (blue dashed line) and ϵ (red solid line). N is the number of open channels in each sector of k_z, k_0 space.

inverse lifetime as a function of k_z for three different values of R for $\epsilon = 12$. In Fig. 5 we plot Γ/Ω vs k_z. One can see that near annihilation the dependence exhibits two minima which correspond to the pair of BSCs with the opposite winding number. In the leading term the dependance could be approximated as

$$\Gamma \sim (k_z - k_z^{\rm BSC})^2 (k_z + k_z^{\rm BSC})^2, \tag{18}$$

where $\pm k_z^{\rm BSC}$ is the position of the minima. In the annihilation point $k_z^{\rm BSC} = 0$ according to Eq. (18) we have $\Gamma \sim k_z^4$, which complies with the recent findings by Yuan and Lu [21] who produced the same asymptotic behavior for standing wave BSCs unprotected by symmetry. The

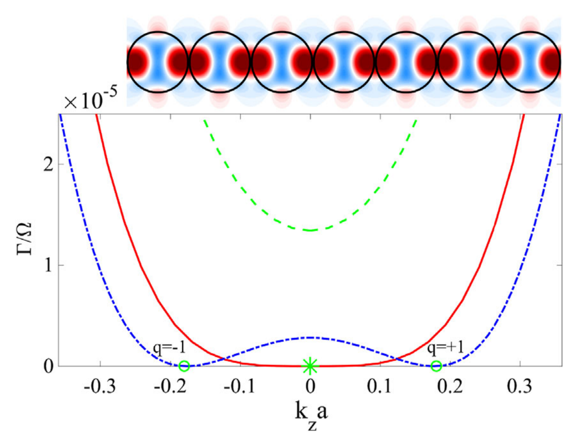

FIG. 5. The inverse lifetime Γ against k_z in the vicinity of the annihilation point. The BSCs approach annihilation at $R = 0.487a$, blue dashed-dotted line; annihilation, standing wave BSC emerges at $R = 0.490a$, solid red line; the BSCs are destroyed at $R = 0.491a$, dashed green line. The field pattern H_z of the standing wave BSC in the $y0z$ plane is shown on top.

field pattern of that BSC is shown on top of Fig. 5 where one can see that the BSC is not symmetry protected.

In summary, we have demonstrated that the Bloch BSCs in periodic arrays of dielectric spheres are associated with a phase singularity of the quasimode coupling strength $\mathcal{W}_s$. That makes such BSCs topologically protected and robust against any variation of parameters preserving the periodicity and rotational symmetry about the array axis. It is demonstrated that the Bloch BSCs can be only destroyed by either annihilation in $k_z = 0$ or by migration to the sector of k_0, k_z space where the second radiation channel is open. Importantly, according to Ref. [22] $\mathcal{W}_s$ is directly related to the scattering cross section. It was demonstrated in Ref. [23] that in the parametric vicinity of a Bloch BSC the singular quasimode dominates the near-field resonant response. Meanwhile, in the far field the phase of the resonant term in Eq. (9) controls the interference between the scattered wave and the background impinging wave to form a Fano feature which is recognized as a hallmark of phase singularities in the scattering cross section [24]. In the recent years we have seen a surge of interest to topological light [25] including topological states in arrays of dielectric nanoparticles [26]. The quasimodal expansion is a natural instrument for describing optical systems with radiative (non-Hermitian) boundary conditions [18]. We conjecture that the proposed approach linking quasimodes to the topological charge could be universal for Bloch BSCs in periodic dielectric structures.

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