Conditional robustness of propagating bound states in the continuum on biperiodic structures

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Abstract

For a periodic structure sandwiched between two homogeneous media, a bound state in the continuum (BIC) is a guided Bloch mode with a frequency in the radiation continuum. Optical BICs have found many applications, mainly because they give rise to resonances with ultra-high quality factors. If the periodic structure has a relevant symmetry, a BIC may have a symmetry mismatch with incoming and outgoing propagating waves of the same frequency and compatible wavevectors, and is considered as protected by symmetry. Propagating BICs with nonzero Bloch wavevectors have been found on many highly symmetric periodic structures. They are not protected by symmetry in the usual sense (i.e., there is no symmetry mismatch), but some of them seem to depend on symmetry for their existence and robustness. In this paper, we show that the low-frequency propagating BICs (with only one radiation channel) on biperiodic structures with an inversion symmetry in the plane of periodicity and a reflection symmetry in the perpendicular direction are robust to symmetry-preserving structural perturbations. In other words, a propagating BIC continues its existence with a slightly different frequency and a slightly different Bloch wavevector, when the biperiodic structure is perturbed slightly preserving the inversion and reflection symmetries. Our study enhances theoretical understanding for BICs on periodic structures and provides useful guidelines for their applications.
I. INTRODUCTION

A bound state in the continuum (BIC) is a trapped or guided mode with a frequency in the frequency interval where incoming and outgoing propagating waves (with compatible wavevectors, when appropriate) exist \[1\). Mathematically, a BIC corresponds to a discrete eigenvalue in the continuous spectrum, and causes the nonuniqueness of a corresponding scattering or diffraction problem \[4, 5\]. It is known that BICs can exist on different configurations including waveguides with local distortions \[6, 7\], waveguides with lateral leaky structures \[8, 10\], waveguides with anisotropic materials \[11\], and periodic structures surrounded by or sandwiched between homogeneous media \[4, 5, 12–32\]. On structures with a relevant symmetry, there can be symmetry-protected BICs that do not couple with the incoming and outgoing propagating waves due to a symmetry mismatch \[4–6, 12–16\]. The more intricate BICs are those without the usual symmetry protection (i.e., there is no symmetry mismatch) \[17–30\]. Related to a BIC on a periodic structure, diffraction problems for given incident waves exhibit interesting properties such as nonuniqueness, total and zero reflection or transmission, and discontinuities in transmission and reflection coefficients \[4, 28, 33, 34\]. A BIC can also be regarded as a resonant mode with an infinite quality factor (\(Q\)-factor). This implies that resonant modes with extremely large \(Q\)-factors can be created by perturbing the structure or varying a physical parameter slightly \[35–39\]. Because of these properties, optical BICs have found applications in lasing \[40, 41\], sensing \[42, 43\], filtering \[44, 45\], and switching \[46\], and can be used to enhance emissive processes and nonlinear optical effects \[47, 48\].

Theoretical questions concerning the BICs include their existence, robustness, and disappearance (becoming resonances). The existence of symmetry-protected BICs can be established rigorously \[4, 6, 14\]. These BICs are also robust against small structural perturbations that preserve the relevant symmetry. If the perturbed structure breaks the symmetry, a symmetry-protected BIC usually turns to a resonant mode with a \(Q\)-factor proportional to \(1/\delta^2\), where \(\delta\) is the strength of the perturbation, but under special conditions, the \(Q\)-factor can be \(O(1/\delta^4)\) or even \(O(1/\delta^6)\) \[39\]. The case for BICs without the usual symmetry protection is more complicated. Many of these BICs are found on highly symmetric structures for relatively low frequencies such that there is only one radiation channel \[1, 20, 22, 28\]. It is certainly possible for BICs to exist on structures without any symmetry and for higher
frequencies with more than one radiation channels, but they are more difficult to find, and usually require the tuning of more parameters. While the numerical results and experimental evidences for BICs unprotected by symmetry are very convincing, to the best of our knowledge, there is no rigorous proof for their existence. Numerical studies also reveal that those BICs on highly symmetric periodic structures are robust to changes in parameters, such as the radius of air holes or dielectric rods or spheres, dielectric constants of the components, and the thickness of the structure \[21, 49, 50\]. It has been realized that although these BICs are not protected by symmetry in the usual sense, symmetry still plays a key role for their continual existence \[20\]. In \[51\], we analyzed this problem for 2D structures with reflection symmetries in both the periodic and perpendicular directions, and showed that the low-frequency BICs (unprotected by symmetry, with only one radiation channel) are robust to any symmetry-preserving perturbations. Due to the conditions imposed on the original and perturbed structures and the BIC, the robustness is only conditional. Furthermore, if the perturbation (of strength \(\delta\)) breaks the relevant symmetry, a BIC (unprotected by symmetry) usually turns to a resonant mode with a \(Q\)-factor proportional to \(1/\delta^2\). Under special conditions, the \(Q\)-factor can be proportional to \(1/\delta^4\) \[39\].

As an extension of our previous work on 2D structures \[51\], we analyze propagating BICs on lossless biperiodic structures sandwiched between two identical homogeneous media in this paper. The structures are assumed to have an inversion symmetry in the plane of periodicity and a reflection symmetry in the perpendicular direction. A propagating BIC has a nonzero Bloch wavevector and is unprotected by symmetry. We show that any low-frequency propagating BIC (with only one radiation channel) on such a biperiodic structure is robust against any lossless structural perturbations that preserve the inversion and reflection symmetries. In other words, if the strength \(\delta\) of the symmetry-preserving perturbation is sufficiently small, the perturbed structure has a BIC with a slightly different frequency and a slightly different Bloch wavevector. This conditional robustness result is established using a perturbation method where the frequency, Bloch wavevector and the field of the BIC on the perturbed structure are expanded as power series of \(\delta\).

The rest of this paper is organized as follows. In Sec. II, we describe the biperiodic structure and recall the basic equations. In Sec. III, we construct special diffraction solutions with desirable symmetry properties. In Sec. IV, we scale the BICs and reveal their symmetry properties. These regularized diffraction solutions and BICs are used in Sec. V to establish
the conditional robustness. The paper is concluded with some discussion in Sec. VI.

II. STRUCTURES AND EQUATIONS

We consider a three-dimensional (3D) isotropic and lossless structure that is periodic in the $x$ and $y$ directions with period $L$, has a finite size $2d$ in the $z$ direction, and is sandwiched between two identical homogeneous media of dielectric constant $\varepsilon_0$. The dielectric function $\varepsilon(\mathbf{x})$, for $\mathbf{x} = (x, y, z)$, of the structure and the surrounding media, is real, satisfies $\varepsilon(\mathbf{x}) = \varepsilon_0$ for $|z| > d$ and

$$\varepsilon(\mathbf{x}) = \varepsilon(x + mL, y + nL, z)$$

for all integers $m$ and $n$. In addition to the periodicity, we assume the structure has a reflection symmetry in the $z$-direction and an inversion symmetry in the $xy$ plane, i.e

$$\varepsilon(\mathbf{x}) = \varepsilon(x, y, -z) = \varepsilon(-x, -y, z).$$

For isotropic, lossless and non-magnetic 3D structures, time-harmonic electromagnetic waves satisfy the following Maxwell’s equations

$$\nabla \times E = i\omega\mu_0 H,$$ 

$$\nabla \times H = -i\omega\varepsilon_0 \varepsilon E,$$

$$\nabla \cdot (\varepsilon E) = 0,$$

$$\nabla \cdot H = 0,$$

where $E$ and $H$ are the electric and magnetic fields respectively, $\omega$ is the angular frequency, $\mu_0$ is the permeability of vacuum, and $\varepsilon_0$ is the permittivity of vacuum. The time dependence is assumed to be $e^{-i\omega t}$ and is already separated. Eliminating $H$, one obtains

$$\nabla \times \nabla \times E - k^2 \varepsilon E = \nabla(\nabla \cdot E) - \nabla^2 E - k^2 \varepsilon E = 0,$$

where $k = \omega/c$ is the freespace wavenumber and $c$ is the speed of light in vacuum. If the electric field is known, the magnetic field can be easily obtained from Eq. (3).

III. DIFFRACTION SOLUTIONS

In this section, we consider diffraction problems with given incident plane waves. The main purpose is to construct diffraction solutions with some desirable symmetry properties.
These solutions will be used in a perturbation process to establish the conditional robustness of propagating BICs. In the homogeneous media below \((z < -d)\) and above \((z > d)\) the structure, we specify plane incident waves

\[ E^{(\text{in})}_\pm(x) = f^\pm e^{i k^\pm \cdot x}, \quad \mp z > d, \tag{8} \]

where \(k^\pm = (\alpha, \beta, \pm \gamma)\) are real wavevectors satisfying \(\|k^\pm\|^2 = k^2 \varepsilon_0\) and \(\gamma > 0\), and \(f^\pm = (f_x, f_y, \pm f_z)\) are real vectors satisfying \(\|f^\pm\| = 1\). In addition, Eq. (5) in the homogeneous media gives the orthogonality condition

\[ f^\pm \cdot k^\pm = 0. \]

We assume the frequency and the wavevectors satisfy

\[ \sqrt{\alpha^2 + \beta^2} < k \sqrt{\varepsilon_0} < \min \left\{ \sqrt{\alpha^2 + (2\pi/L - |\beta|)^2}, \sqrt{(2\pi/L - |\alpha|)^2 - \beta^2} \right\}. \tag{9} \]

This implies that the \((0,0)\)-th order diffraction channel is the only propagating channel. More precisely, let

\[ \hat{\alpha}_j = \alpha + 2j\pi/L, \quad \hat{\beta}_m = \beta + 2m\pi/L, \quad \hat{\gamma}_{jm} = \sqrt{k^2 \varepsilon_0 - \hat{\alpha}_j^2 - \hat{\beta}_m^2} \tag{10} \]

for all integers \(j\) and \(m\), where \(\hat{\alpha}_0 = \alpha, \hat{\beta}_0 = \beta\) and \(\hat{\gamma}_{00} = \gamma\), then only \(\hat{\gamma}_{00}\) is real and all other \(\hat{\gamma}_{jm}\) for \((j, m) \neq (0, 0)\) are pure imaginary.

Let \(\tilde{E}_e(x) = [\tilde{E}_{e,x}(x), \tilde{E}_{e,y}(x), \tilde{E}_{e,z}(x)]\) be a solution of the diffraction problem with incident plane waves given in Eq. (8). Since the structure has a reflection symmetry in the \(z\)-direction, the vector field

\[ \hat{E}_e(x) = \left[ \tilde{E}_{e,x}(x, y, -z), \tilde{E}_{e,y}(x, y, -z), -\tilde{E}_{e,z}(x, y, -z) \right] \]

also satisfies Eqs. (7) and (5). In addition, the set of two incident plane waves given in Eq. (8) is unchanged if we map \(z\) to \(-z\) and multiply \(-1\) to their \(z\)-components. Thus, \(\tilde{E}_e(x)\) solves the same diffraction problem. If this diffraction problem has a unique solution, then \(\tilde{E}_e(x) = \hat{E}_e(x)\). If the diffraction problem does not have a unique solution, we can still assume \(\tilde{E}_e(x) = \hat{E}_e(x)\), because otherwise we can replace \(\tilde{E}_e(x)\) by \([\hat{E}_e(x) + \tilde{E}_e(x)]/2\) which solves the same diffraction problem. The condition \(\tilde{E}_e(x) = \hat{E}_e(x)\) implies that the \(x\) and \(y\) components of \(\tilde{E}_e\) are even in \(z\) and the \(z\) component of \(\tilde{E}_e\) is odd in \(z\), i.e.,

\[ \tilde{E}_{e,x}(x) = \tilde{E}_{e,x}(x, y, -z), \quad \tilde{E}_{e,y}(x) = \tilde{E}_{e,y}(x, y, -z), \quad \tilde{E}_{e,z}(x) = -\tilde{E}_{e,z}(x, y, -z). \tag{11} \]
Since the media for $|z| > d$ are homogeneous and the $(0,0)$-th order diffraction channel is the only propagating channel, $\tilde{E}_e(x)$ has the following asymptotic formula

$$\tilde{E}_e(x) \sim f^+ e^{ik^+ \cdot x} + g^\pm e^{ik^\pm \cdot x}, \quad z \to \pm \infty.$$  \hfill (12)

where $g^\pm$ are the constant vectors for the outgoing plane waves. Due to the symmetry given in condition (11), the $x$- and $y$-components of $g^\pm$ are identical respectively, and their $z$-components have opposite signs. In addition, $g^\pm$ must satisfy $g^\pm \cdot k^\pm = 0$ due to Eq. (5), and $\|g^\pm\| = 1$ due to energy conservation.

Notice that $\overline{\tilde{E}_e(-x)}$, i.e. the complex conjugate of $\tilde{E}_e(-x)$, also satisfies Eqs. (7) and (5), and has the asymptotic formula

$$\overline{\tilde{E}_e(-x)} \sim \overline{g}^\mp e^{ik^\mp \cdot x} + \overline{f}^\pm e^{ik^\pm \cdot x}, \quad z \to \pm \infty.$$  \hfill (13)

Therefore, $\overline{\tilde{E}_e(-x)}$ can be regarded as a solution of the diffraction problem with incident plane waves $\overline{g}^\mp e^{ik^\mp \cdot x}$. If $f^- + \overline{g}^- \neq 0$, we let $E_e(x) = \tilde{E}_e(x) + \overline{\tilde{E}_e(-x)}$, then $E_e$ satisfies the parity-time ($\mathcal{PT}$) symmetry condition

$$E_e(x) = \overline{E_e(-x)}.$$  \hfill (13)

The asymptotic formula of $E_e(x)$ at infinity can be written as

$$E_e(x) \sim \begin{cases} c^- e^{ik^- \cdot x} + \overline{c}^+ e^{ik^+ \cdot x}, & z \to +\infty, \\ c^+ e^{ik^+ \cdot x} + \overline{c}^- e^{ik^- \cdot x}, & z \to -\infty, \end{cases} \hfill (14)$$

where $c^\pm = f^\pm + \overline{g}^\pm$. It is easy to verify that $\|c^-\| = \|c^+\|$, the $x$- and $y$-components of $c^\pm$ are identical respectively, and the $z$-components have opposite signs. We can scale $E_e$ such that $\|c^\pm\| = 1$. If $f^- + \overline{g}^- = 0$, then $E_e = i\tilde{E}_e$ is a solution of a diffraction problem with incident plane waves $i f^\pm e^{ik^\pm \cdot x}$. In that case, conditions (13) and (14) are still valid with $c^\pm = i f^\pm$. In summary, we have constructed a diffraction solution $E_e$ which satisfies conditions (11) and (13).

Similarly, for incident plane waves

$$E_e^{(in)}(x) = \frac{k^- \times f^-}{\|k^- \times f^-\|} e^{ik^- \cdot x}, \quad E_e^{(in)}(x) = -\frac{k^+ \times f^+}{\|k^+ \times f^+\|} e^{ik^+ \cdot x},$$  \hfill (15)

given in the media for $z > d$ and $z < -d$, respectively, we can construct a diffraction solution $E_e^{(2)}(x)$ by following the same procedure above. The solution $E_e^{(2)}(x)$ satisfies the symmetry
conditions (11) and (13). The asymptotic formula of \( E^{(2)}_e(x) \) at infinity is

\[
E^{(2)}_e(x) \sim \begin{cases} 
  v^- e^{ik^- x} + \nabla^+ e^{ik^+ x}, & z \to +\infty, \\
  v^+ e^{ik^+ x} + \nabla^- e^{ik^- x}, & z \to -\infty,
\end{cases}
\]

where \( v^\pm \) are defined by the same procedure as \( c^\pm \) and scaled such that \( \|v^\pm\| = 1 \). It is easy to show that \( v^\pm \cdot k^\pm = 0 \) and \( v^\pm \cdot c^\pm = 0 \). Therefore, the vectors \( k^+, c^+, v^+ \) form an orthonormal basis in the 3D space.

If we replace \( f^- \) by \( -f^- \) and follow the same procedure above, we can construct diffraction solutions \( E_o(x) \) and \( E^{(2)}_o(x) \) that satisfy the same \( \mathcal{PT} \)-symmetry condition (13) and the following condition

\[
E_{o,x}(x) = -E_{o,x}(x, y, -z), \quad E_{o,y}(x) = -E_{o,y}(x, y, -z), \quad E_{o,z}(x) = E_{o,z}(x, y, -z).
\]

In other words, the \( x \)- and \( y \)-components of \( E_o \) (or \( E^{(2)}_o \)) are odd in \( z \) and the \( z \)-component of \( E_o \) (or \( E^{(2)}_o \)) is even in \( z \).

Since the structure is periodic in \( x \) and \( y \) with period \( L \), a diffraction solution can be written as a Bloch wave

\[
E_e(x) = e^{ib \cdot x} \Psi_e(x) \quad \text{for} \quad b = (\alpha, \beta, 0),
\]

where \( \Psi_e(x) \) is periodic in \( x \) and \( y \) with period \( L \) and satisfies the same symmetry conditions as \( E_e(x) \), i.e. (11) and (13). In terms of \( \Psi_e(x) \), the governing equations (7) and (5) become

\[
(\nabla + ib) \times (\nabla + ib) \times \Psi_e - k^2 \varepsilon \Psi_e = 0,
\]

\[
(\nabla + ib) \cdot (\varepsilon \Psi_e) = 0.
\]

Similarly, we can introduce functions \( \Theta_e(x), \Psi_o(x) \) and \( \Theta_o(x) \) such that

\[
E_o(x) = e^{ib \cdot x} \Psi_o(x), \quad E^{(2)}_e(x) = e^{ib \cdot x} \Theta_e(x), \quad E^{(2)}_o(x) = e^{ib \cdot x} \Theta_o(x).
\]

These functions are periodic in \( x \) and \( y \) with period \( L \), satisfy Eqs. (19) and (20), and the same symmetry conditions as \( E^{(2)}_e(x) \), \( E_o(x) \) and \( E^{(2)}_o(x) \), respectively.

IV. BOUND STATES IN THE CONTINUUM

A Bloch mode on a biperiodic structure sandwiched between two homogeneous media is a solution of Eqs. (7) and (5) given as

\[
E(x) = e^{i(\alpha x + \beta y)} \Phi(x, y, z) = e^{ib \cdot x} \Phi(x),
\]
where \( \Phi(x) \) is periodic in \( x \) and \( y \) with period \( L \) and satisfies Eqs. (19) and (20), and \( \mathbf{b} = (\alpha, \beta, 0) \) is the Bloch wavevector. A Bloch mode is a guided (or localized) mode if \( (\alpha, \beta) \) is a real pair and \( \Phi \to 0 \) as \( |z| \to \infty \). Typically, guided modes that depend on \( (\alpha, \beta) \) and \( \omega \) continuously can be found below the light cone, i.e. for \( k \sqrt{\varepsilon_0} < \sqrt{\alpha^2 + \beta^2} \). Guided modes may also exist in the light cone, i.e. for \( k \sqrt{\varepsilon_0} > \sqrt{\alpha^2 + \beta^2} \). This is true especially when the structure has certain symmetry. Such a guided mode in the light cone is a bound states in the continuum (BIC).

Since the media for \( |z| > d \) are homogeneous, a Bloch mode can be expanded as

\[
E(x) = \sum_{j,m=-\infty}^{+\infty} a_{jm}^\pm e^{ik_{jm} \cdot x}, \quad |z| > d, \tag{23}
\]

where the “+” and “−” signs correspond to \( z > d \) and \( z < -d \), respectively, and

\[
k_{jm}^\pm = \left( \hat{\alpha}_j, \hat{\beta}_m, \pm \hat{\gamma}_{jm} \right). \tag{24}
\]

Equation (5) requires that \( k_{jm}^\pm \cdot a_{jm}^\pm = 0 \) for all integers \( j \) and \( m \). If \( \omega \) is real and \( \alpha_j^2 + \beta_m^2 > k^2 \varepsilon_0 \), then \( \hat{\gamma}_{jm} \) is pure imaginary, and the corresponding plane wave is evanescent. For a BIC, all coefficients \( a_{jm}^\pm \) corresponding to real \( \hat{\gamma}_{jm} \) must vanish, since the field must decay to zero as \( |z| \to \infty \). If condition (9) is satisfied, only \( \gamma = \hat{\gamma}_{00} \) is real and all other \( \hat{\gamma}_{jm} \) for \( (j, m) \neq (0, 0) \) are pure imaginary. In that case, the Bloch mode is a BIC if and only if \( a_{00}^\pm = 0 \).

On biperiodic structures with an inversion symmetry in the \( xy \) plane, i.e. \( \varepsilon(x) = \varepsilon(-x, -y, z) \), there may exist symmetry-protected BICs with \( \alpha = \beta = 0 \), and they satisfy

\[
E_x(x) = -E_x(-x, -y, z), \quad E_y(x) = -E_y(-x, -y, z), \quad E_z(x) = E_z(-x, -y, z). \tag{25}
\]

The above condition forces the \( x- \) and \( y- \)components of \( a_{00}^\pm \) to vanish, but since \( k_{00}^\pm \cdot a_{00}^\pm = 0 \), the \( z- \)components of \( a_{00}^\pm \) are zero. Therefore, if condition (9) is satisfied, a Bloch mode (with \( \alpha = \beta = 0 \)) satisfying condition (25) is always a BIC. Notice that the reflection symmetry in \( z \) is not required for the existence of these symmetry-protected BICs.

For propagating BICs, we assume condition (2) is satisfied, i.e., the structure has an inversion symmetry in the \( xy \) plane and a reflection symmetry in \( z \). If \( E(x) \) is a propagating BIC, then

\[
\hat{E}(x) = \begin{bmatrix} E_x(x, y, -z), & E_y(x, y, -z), & -E_z(x, y, -z) \end{bmatrix} \tag{26}
\]
is also a BIC with the same Bloch wavevector and the same frequency. We can assume the BIC satisfies either

\[ E_x(x) = E_x(x, y, -z), \quad E_y(x) = E_y(x, y, -z), \quad E_z(x) = -E_z(x, y, -z), \quad (27) \]

or

\[ E_x(x) = -E_x(x, y, -z), \quad E_y(x) = -E_y(x, y, -z), \quad E_z(x) = E_z(x, y, -z), \quad (28) \]

since otherwise, it can be replaced by \[ \frac{E(x) + \hat{E}(x)}{2} \] or \[ \frac{E(x) - \hat{E}(x)}{2} \]. Notice that the vector function \( \Phi(x) \) given in Eq. (22) also satisfies (27) or (28).

If \( E(x) \) is a BIC, it is easy to show that \( \mathbf{E}(-x) \) is also a BIC with the same frequency and the same Bloch wavevector. Assuming the BIC is non-degenerate (i.e. single), then there must be a constant \( \rho \) such that \( E(x) = \rho \mathbf{E}(-x) \). Evaluating the energy of the BIC on one period of the structure, we conclude that \( \rho \) must satisfy \( |\rho| = 1 \). Let \( \rho = e^{2i\theta} \), then \( W(x) = e^{-i\theta} E(x) \) is also a BIC and \( W(x) = \overline{W}(-x) \). Therefore, without loss of generality, we can assume the propagating BIC satisfies

\[ E(x) = \overline{E}(-x), \quad (29) \]

i.e., it is \( \mathcal{PT} \)-symmetric. In that case, the vector function \( \Phi(x) \) given in Eq. (22) is also \( \mathcal{PT} \)-symmetric.

V. CONDITIONAL ROBUSTNESS OF PROPAGATING BICS

In this section, we establish a conditional robustness for some propagating BICS on some biperiodic structures. The robustness of a BIC refers to its continual existence under small structural perturbations. It should be emphasized that the robustness is only conditional, because there are conditions on the original biperiodic structure, the structural perturbation, and the BIC itself. More specifically, the biperiodic structure is required to satisfy the conditions specified in Sec. III. Importantly, it must have an inversion symmetry in the \( xy \) plane and a reflection symmetry along the \( z \) axis. The BIC must be non-degenerate, must have a Bloch wavevector \( b = (\alpha, \beta, 0) \neq 0 \) and a frequency \( \omega \) (or freespace wavenumber \( k \)) satisfying condition (9), and must satisfy \( \det(A) \neq 0 \) for the matrix \( A \) given below. Without loss of generality, we assume the BIC satisfies symmetry condition (27), that is, its \( x \) and
$y$ components are even in $z$ and its $z$ component is odd in $z$. The dielectric function of a perturbed structure is given by

$$\tilde{\varepsilon}(\mathbf{x}) = \varepsilon(\mathbf{x}) + \delta s(\mathbf{x}), \quad (30)$$

where $\delta$ is a small real number, $s(\mathbf{x})$ is any $O(1)$ real function satisfying $s(\mathbf{x}) = 0$ for $|z| > d$, the periodic condition (I) and the symmetry condition (II). Under these conditions, we claim that for any sufficiently small $\delta$, the perturbed structure has a BIC with a frequency $\tilde{\omega}$ near $\omega$ and a Bloch wavevector $\tilde{\mathbf{b}} = (\tilde{\alpha}, \tilde{\beta}, 0)$ near $\mathbf{b}$. Although the perturbation profile $s(\mathbf{x})$ must preserve the periodicity and the inversion and reflection symmetries, it can still be quite arbitrary, therefore, our robustness result is a general result.

To establish the conditional robustness, we construct a BIC on the perturbed structure using a perturbation method. Let $E(\mathbf{x}) = e^{i(\alpha x + \beta y)}\Phi(\mathbf{x})$ be a BIC on the original biperiodic structure, where $\Phi(\mathbf{x})$ is periodic in $x$ and $y$ with period $L$ and tends to zero exponentially as $|z| \to \infty$, we look for a BIC $\tilde{E}(\mathbf{x}) = e^{i(\tilde{\alpha} x + \tilde{\beta} y)}\tilde{\Phi}(\mathbf{x})$ on the perturbed structure by expanding $\tilde{\Phi}$, $\tilde{k}$, $\tilde{\alpha}$ and $\tilde{\beta}$ in power series of $\delta$

$$\tilde{\Phi}(\mathbf{x}) = \Phi(\mathbf{x}) + \delta \Phi_1(\mathbf{x}) + \delta^2 \Phi_2(\mathbf{x}) + \ldots, \quad (31)$$

$$\tilde{k} = k + \delta k_1 + \delta^2 k_2 + \ldots, \quad (32)$$

$$\tilde{\alpha} = \alpha + \delta \alpha_1 + \delta^2 \alpha_2 + \ldots, \quad (33)$$

$$\tilde{\beta} = \beta + \delta \beta_1 + \delta^2 \beta_2 + \ldots. \quad (34)$$

The last two expansions above can be written as

$$\tilde{\mathbf{b}} = \mathbf{b} + \delta \mathbf{b}_1 + \delta^2 \mathbf{b}_2 + \ldots \quad (35)$$

where $\mathbf{b}_j = (\alpha_j, \beta_j, 0)$ for $j \geq 1$. In the following, we show that for each $j \geq 1$, $\Phi_j(\mathbf{x})$ can be solved, it is periodic in $x$ and $y$ with period $L$ and decays to zero exponentially as $z \to \infty$, $k_j$, $\alpha_j$ and $\beta_j$ can be determined and they are all real numbers.

Substituting expansions (31), (32) and (35) into Eqs. (19) and (20), and comparing the coefficients of $\delta^j$ for $j \geq 1$, we obtain the following equations for $\Phi_j$:

$$\mathcal{L}\Phi_j = \alpha_j \mathcal{B}_1 \Phi + \beta_j \mathcal{B}_2 \Phi + 2kk_j \varepsilon \Phi + F_j, \quad (36)$$

$$\nabla(\varepsilon \Phi_j) = \alpha_j p_1 + \beta_j p_2 + g_j, \quad (37)$$
respectively, and

\[ \mathcal{L} = (\nabla + i\mathbf{b}) \times (\nabla + i\mathbf{b}) \times -k^2\varepsilon, \]  

(38)

\[ B_m = -i [\nabla \times \mathbf{e}_m \times +\mathbf{e}_m \times \nabla \times] + \mathbf{e}_m \times \mathbf{b} \times +\mathbf{b} \times \mathbf{e}_m \times, \]  

(39)

\[ p_m = -i\varepsilon \mathbf{e}_m \cdot \Phi \]  

(40)

for \( m = 1 \) and 2, \( \mathbf{e}_1 = (1, 0, 0) \) and \( \mathbf{e}_2 = (0, 1, 0) \) are unit vectors along the \( x \) and \( y \) axes, respectively, and

\[ F_1 = sk^2\Phi, \quad g_1 = -\nabla \cdot (s\Phi), \]

and for \( j > 1, \)

\[ F_j = -i \sum_{m=1}^{j-1} [\nabla \times (b_{j-m} \times \Phi_m) + b_{j-m} \times (\nabla \times \Phi_m)] + \sum_{m=1}^{j-1} \sum_{n=0}^{j-m} b_{j-m-n} \times (b_n \times \Phi_m) \]

\[ + \sum_{m=1}^{j-1} b_{j-m} \times (b_m \times \Phi) + \sum_{m=1}^{j-1} \left[ \varepsilon \sum_{n=0}^{j-m} k_{j-m-n} k_n + s \sum_{n=0}^{j-m-1} k_{j-m-n} k_n \right] \Phi_m \]

\[ + \varepsilon \sum_{m=1}^{j-1} k_{j-m} k_m \Phi + s \sum_{m=0}^{j-1} k_{j-m} k_m \Phi, \]

\[ g_j = -\nabla \cdot (s\Phi_{j-1}) - isb_{j-1} \cdot \Phi - i \sum_{n=1}^{j-1} (\varepsilon b_{j-n} + sb_{j-n-1}) \cdot \Phi_n \]

In the above, \( \alpha_0 = \alpha, \beta_0 = \beta, k_0 = k \) and \( \Phi_0 = \Phi. \) Notice that \( \mathcal{L}, B_1 \) and \( B_2 \) are operators, \( p_1 \) and \( p_2 \) are scalar functions, and all of them are independent of \( j. \) Moreover, \( F_j \) is a vector function, \( g_j \) is a scalar function, and they do not involve \( \alpha_j, \beta_j, k_j \) and \( \Phi_j. \)

In the \( j \)-th step, we need to determine \( \alpha_j, \beta_j \) and \( k_j, \) and a vector function \( \Phi_j \) which is periodic in \( x \) and \( y \) and decays to zero exponentially as \( |z| \to \infty. \) First, we show that if Eqs. \( 36 \) and \( 37 \) have such a solution \( \Phi_j, \) then \( \alpha_j, \beta_j \) and \( k_j \) must satisfy the following linear system

\[ \mathbf{A} \begin{bmatrix} \alpha_j \\ \beta_j \\ k_j \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} \alpha_j \\ \beta_j \\ k_j \end{bmatrix} = \begin{bmatrix} b_{1j} \\ b_{2j} \\ b_{3j} \end{bmatrix}, \]  

(41)

where

\[ a_{1m} = \int_\Omega \overline{\Phi} \cdot B_m \Phi dx, \quad a_{13} = 2k \int_\Omega \varepsilon \overline{\Phi} \cdot \Phi dx, \]

(42)

\[ a_{2m} = \int_\Omega \overline{\mathbf{e}} \cdot B_m \Phi dx, \quad a_{23} = 2k \int_\Omega \varepsilon \overline{\mathbf{e}} \cdot \Phi dx, \]

(43)

\[ a_{3m} = \int_\Omega \overline{\mathbf{e}} \cdot B_m \Phi dx, \quad a_{33} = 2k \int_\Omega \varepsilon \overline{\mathbf{e}} \cdot \Phi dx, \]

(44)
for $m = 1, 2$, $\Psi_e$ and $\Theta_e$ are related to diffraction solutions $E_e$ and $E_e^{(2)}$ introduced in Sec. III:

\[ b_{1j} = -\int_{\Omega} \Phi \cdot F_j dx, \quad b_{2j} = -\int_{\Omega} \Psi_e \cdot F_j dx, \quad b_{3j} = -\int_{\Omega} \Theta_e \cdot F_j dx, \quad (45) \]

and $\Omega$ is the 3D domain given by $|x| < L/2$, $|y| < L/2$ and $|z| < +\infty$. This linear system is obtained by computing the dot products of Eq. (36) with $\Phi$, $\Psi_e$ and $\Theta_e$, respectively, integrating the results on domain $\Omega$, and showing that left hand sides are all zero (as in Appendix A). Therefore, the three equations in system (41) are actually

\[ \int_{\Omega} \Phi \cdot (\alpha_j B_m \Phi + \beta_j B_m \Phi + 2kk_j \phi \Phi + F_j) = 0, \quad (46) \]

\[ \int_{\Omega} \Psi_e \cdot (\alpha_j B_m \Phi + \beta_j B_m \Phi + 2kk_j \phi \Phi + F_j) = 0, \quad (47) \]

\[ \int_{\Omega} \Theta_e \cdot (\alpha_j B_m \Phi + \beta_j B_m \Phi + 2kk_j \phi \Phi + F_j) = 0. \quad (48) \]

Although $\alpha_j$, $\beta_j$ and $k_j$ can be solved from system (41) if det($A$) $\neq 0$, it is still necessary to show that Eqs. (36) and (37) indeed have a solution $\Phi_j$. In the following, we show that if $A$ is invertible, then $\alpha_j$, $\beta_j$ and $k_j$ are real, and Eqs. (36) and (37) have a solution $\Phi_j$ that is periodic in $x$ and $y$ with period $L$, decays exponentially as $|z| \rightarrow \infty$, is $PT$-symmetric, and satisfies the same symmetry condition in $z$ [assumed to be (27)] as the BIC.

For the case $j = 1$, since $\Phi$, $\Psi_e$, $\Theta_e$, $B_m \Phi$ and $F_1 = sk^2 \Phi$ are all $PT$-symmetric, the coefficient matrix $A$ and the right hand side of linear system Eq. (41) are real. Therefore, if det($A$) $\neq 0$, $\alpha_1$, $\beta_1$ and $k_1$ can be uniquely solved from Eq. (41), and they are real. The BIC satisfies $L\Phi = 0$, thus the inhomogeneous equation (36) for $\Phi_j$ is singular. In general, such a singular inhomogeneous equation does not have a solution unless its right hand side is orthogonal with the nullspace of $L$. We have assumed that the BIC is non-degenerate. Therefore, Eq. (36) has solutions if its right hand side is orthogonal with $\Phi$, that is, if condition (46) is satisfied. For the case $j = 1$, it is clear that the right hand side decays to zero as $|z| \rightarrow \infty$. Therefore, it is natural to require $\Phi_1$ to satisfy outgoing radiation condition as $z \rightarrow \pm \infty$. Since there is only one opening diffraction channel, $\Phi_1$ has an asymptotic formula at infinity

\[ \Phi_1(x) \sim d^\pm e^{\pm i\gamma z}, \quad z \rightarrow \pm \infty, \quad (49) \]

where $d^\pm$ are constant vectors. Since the BIC satisfies the symmetry condition (27), the right hand side of Eq. (36) for $j = 1$ also satisfies (27), and thus we can assume $\Phi_1$ also
satisfies that condition. Therefore, the $x$- and $y$-components of $d^\pm$ are identical, respectively, and their $z$-components have opposite signs.

To show that $\Phi_1$ decays to zero exponentially as $|z| \to +\infty$, we only need to show $d^\pm = 0$. We proceed by taking the dot product of $\overline{\Psi}_e$ with Eq. (36) and integrating the result on domain
\[ \Omega_h = \{(x, y, z) : |x| < L/2, |y| < L/2, |z| < h \} \]
for $h > d$. Using the asymptotic formulae of $\Phi_1$ and $\Psi_e$ at infinity, we can establish the following result
\[ \lim_{h \to \infty} \int_{\Omega_h} \overline{\Psi}_e \cdot \mathcal{L}\Phi_1 d\mathbf{x} = -4i\gamma L^2 \mathbf{c}^+ \cdot \mathbf{d}^+ . \] (50)
A detailed derivation of Eq. (50) is given in Appendix B. On the other hand, according to the second equation of system (41), or Eq. (47),
\[ \lim_{h \to \infty} \int_{\Omega_h} \overline{\Psi}_e \cdot \mathcal{L}\Phi_1 d\mathbf{x} = 0 . \] (51)
Therefore, we must have
\[ \mathbf{c}^+ \cdot \mathbf{d}^+ = 0 . \] (52)
Similarly, taking the dot product of $\overline{\Theta}_e$ with Eq. (36), integrating the result in domain $\Omega_h$, and letting $h \to \infty$, we obtain
\[ \mathbf{v}^+ \cdot \mathbf{d}^+ = 0 . \] (53)
In addition, in the homogeneous medium for $|z| > d$, Eq. (37) leads to $\mathbf{k}^+ \cdot \mathbf{d}^+ = 0$. From Sec III we know that $\{\mathbf{k}^+, \mathbf{c}^+, \mathbf{v}^+\}$ is an orthonormal basis. Therefore, we must have $\mathbf{d}^+ = \mathbf{d}^- = 0$, and thus $\Phi_1$ decays to zero exponentially as $|z| \to +\infty$.

Meanwhile, since $\alpha_1$, $\beta_1$ and $k_1$ are real, it is easy to verify that the right hand side of Eq. (36) for $j = 1$ is $\mathcal{PT}$-symmetric. We can assume $\Phi_1$ is also $\mathcal{PT}$-symmetric, since otherwise we can replace it by $[\Phi_1(x) + \Phi_1(-x)]/2$ which is also a solution of Eqs. (36) and (37).

The same reasoning is applicable to all perturbation steps for $j \geq 2$. More specifically, if $A$ is invertible and the perturbation profile $s(x)$ satisfies symmetry condition (2), and if for all $n < j$, $\alpha_n$, $\beta_n$ and $k_n$ are real, and $\Phi_n$ decays to zero exponentially as $|z| \to \infty$, satisfies symmetry condition (27), and is $\mathcal{PT}$-symmetric, then we can show that $\alpha_j$, $\beta_j$ and $k_j$ are real, and $\Phi_j$ decays to zero exponentially as $|z| \to \infty$, satisfies condition (27), and is $\mathcal{PT}$-symmetric.
If the perturbation profile \( s(x) \) does not satisfy condition Eq. (2), the above perturbation process is likely to fail. In the first step \((j = 1)\), in order to have a real \( b_{21} \), we need to have a real \( \int_\Omega s(x) \overline{\psi} \cdot \Phi \, dx \). This implies that

\[
\int_\Omega [s(x) - s(-x)] \overline{\psi} \cdot \Phi \, dx = 0. \tag{54}
\]

Similarly, \( s(x) \) should satisfy

\[
\int_\Omega [s(x) - s(-x)] \overline{\Theta} \cdot \Phi \, dx = 0. \tag{55}
\]

Moreover, Eqs. (47) and (48) should still hold when \( \psi_e \) and \( \Theta_e \) are replaced by \( \psi_o \) and \( \Theta_o \). Therefore, we must also have \( \int_\Omega s(x) \overline{\psi} \cdot \Phi \, dx = 0 \) and \( \int_\Omega s(x) \overline{\Theta} \cdot \Phi \, dx = 0 \), or

\[
\int_\Omega [s(x) - s(x, y, -z)] \overline{\psi} \cdot \Phi \, dx = \int_\Omega [s(x) - s(x, y, -z)] \overline{\Theta} \cdot \Phi \, dx = 0. \tag{56}
\]

If \( s(x) \) does not satisfy any one of Eqs. (54) - (56), then the perturbation process fails at the first step. If \( s(x) \) satisfies Eqs. (54) - (56), then \( \alpha_1, \beta_1 \) and \( k_1 \) are real, and \( \Phi_1 \) decays to zero exponentially as \( |z| \to +\infty \). At the second step \((j = 2)\), in order to obtain real \( \alpha_2, \beta_2 \) and \( k_2 \), \( s(x) \) must satisfy extra conditions involving \( \Phi_1 \). To carry out the perturbation process successfully for all steps, \( s(x) \) must satisfy an infinite sequence of conditions. Therefore, if \( s(x) \) does not satisfy symmetry condition (2), it is unlikely for the perturbed structure to have a BIC. In that case, the BIC of the original unperturbed structure is turned to a resonant mode with a finite \( Q \)-factor.

VI. CONCLUSION

For biperiodic structures with inversion and reflection symmetries, we showed that the low-frequency propagating BICs (with only one radiation channel) are robust against structural perturbations that preserve the same symmetries. The robustness is only conditional, since a BIC can be easily destroyed by a general perturbation. So far, we have assumed that both the original and the perturbed structure are lossless. It is not difficult to see that the result is still valid if the perturbation profile is symmetric in \( z \) and \( \mathcal{PT} \)-symmetric in \( x \) and \( y \), i.e. \( s(x) = s(x, y, -z) = \overline{s}(-x, -y, z) = \overline{s}(-x) \). A small material loss can also be considered as a perturbation. It is obvious that a lossy biperiodic structure cannot have a BIC with a real frequency and a real Bloch wavenumber. It turns out that it usually cannot even have
a bound state with a complex frequency and a real non-zero Bloch wavevector [52]. In other
words, if the original lossless structure has a propagating BIC and the perturbation profile
$s(x)$ represents material loss and satisfies the symmetry condition [2], then a propagating
BIC is usually destroyed by the perturbation.

The theory developed in this paper is applicable to symmetry-protected BICs, but the
reflection symmetry in $z$ is not necessary. Assuming the biperiodic structure has only the
inversion symmetry in the $xy$ plane, i.e. $\varepsilon(x) = \varepsilon(-x, -y, z)$, a symmetry-protected BIC is
a standing wave (with a zero Bloch wavevector) satisfying

$$E_x(x) = -E_x(-x, -y, z), \quad E_y(x) = -E_y(-x, -y, z), \quad E_z(x) = E_z(-x, -y, z).$$

If we follow the scaling process of Sec. IV, then the electric field $E$ of the symmetry-protected
BIC is pure imaginary. Meanwhile, we can construct two real diffraction solutions $U^{(1)}(x)$
and $U^{(2)}(x)$ for normal incident waves such that

$$U_x^{(l)}(x) = U_x^{(l)}(-x, -y, z), \quad U_y^{(l)}(x) = U_y^{(l)}(-x, -y, z), \quad U_z^{(l)}(x) = -U_z^{(l)}(-x, -y, z)$$

for $l = 1$ and 2. The perturbation process of Sec. V is still valid, provided that we replace
$\Phi, \Psi_e$ and $\Theta_e$ by $E$, $U^{(1)}$ and $U^{(2)}$, respectively. In each step, we can show that $\alpha_j = \beta_j = 0,$
$k_j$ is real, and Eqs. (36) and (37) has a solution $\Phi_j$ that decays to zero exponentially as
$|z| \to +\infty$ and satisfies the same symmetry condition as the BIC.

Finally, we point out that the justification for conditional robustness presented in this
paper is still somewhat informal. It is desirable to develop a rigorous proof, including the
convergence of the series (31) - (34), using a proper functional analysis framework.

ACKNOWLEDGEMENTS

The authors acknowledge support from the Natural Science Foundation of Chongqing,
China (Grant No. cstc2019jcyj-msxmX0717), and the Research Grants Council of Hong
Kong Special Administrative Region, China (Grant No. CityU 11304117).
APPENDIX A

To derive the first equation of the linear system (41), we take the dot product of \( \Phi \) with Eq. (36), integrate on domain \( \Omega = \{ (x, y, z) : |x| < L/2, |y| < L/2, |z| < +\infty \} \), and obtain
\[
\int_{\Omega} \Phi \cdot L\Phi_j \, dx = a_{11}\alpha_j + a_{12}\beta_j + a_{13}k_j - b_{1j}. \tag{57}
\]
We need to show that the left hand side above is zero. Since \( L\Phi = 0 \), we have \( \int_{\Omega} \Phi_j \cdot L\Phi \, dx = 0 \), and thus
\[
\int_{\Omega} \Phi \cdot L\Phi_j \, dx = \int_{\Omega} \left( \Phi \cdot L\Phi_j - \Phi_j \cdot \overline{L}\Phi \right) \, dx = \int_{\Omega} \Phi \cdot (\nabla \times \nabla \times \Phi_j) \, dx + i \int_{\Omega} \Phi \cdot [\nabla \times (b \times \Phi_j)] \, dx + i \int_{\Omega} \Phi \cdot [b \times (\nabla \times \Phi_j)] \, dx
- i \int_{\Omega} \Phi_j \cdot \Phi \times \Phi_j \, dx + i \int_{\Omega} \Phi_j \cdot (\nabla \times \nabla \times \Phi) \, dx + i \int_{\Omega} \Phi_j \cdot [\nabla \times (b \times \Phi)] \, dx
+ i \int_{\Omega} \Phi_j \cdot [b \times (\nabla \times \Phi)] \, dx + i \int_{\Omega} \Phi_j \cdot [b \times (b \times \Phi)] \, dx. \tag{58}
\]
Using the vector identities
\[
A \cdot (\nabla \times B) = B \cdot (\nabla \times A) + \nabla \cdot (B \times A), \tag{59}
A \cdot (B \times C) = B \cdot (C \times A) = C \cdot (A \times B) \tag{60}
\]
in Eq. (58), we have
\[
\int_{\Omega} \Phi \cdot L\Phi_j \, dx = \int_{\Omega} \nabla \cdot [(\nabla \times \Phi_j) \times \Phi] \, dx + i \int_{\Omega} \nabla \cdot [(b \times \Phi_j) \times \Phi] \, dx
- i \int_{\Omega} \nabla \cdot [(\nabla \times \Phi) \times \Phi_j] \, dx + i \int_{\Omega} \nabla \cdot [(b \times \Phi) \times \Phi_j] \, dx.
\]
Because of the Gauss' Law, the above equation becomes
\[
\int_{\Omega} \Phi \cdot L\Phi_j \, dx = \int_{\partial\Omega} \left[ (\nabla \times \Phi_j) \times \Phi \right] \cdot dS + i \int_{\partial\Omega} \left[ (b \times \Phi_j) \times \Phi \right] \cdot dS
- i \int_{\partial\Omega} \left[ (\nabla \times \Phi) \times \Phi_j \right] \cdot dS + i \int_{\partial\Omega} \left[ (b \times \Phi) \times \Phi_j \right] \cdot dS.
\]
Since \( \Phi \) and \( \Phi_j \) are periodic in the \( x \) and \( y \) directions, and \( \Phi \) decays to zero exponentially as \( |z| \to \infty \), the surface integrals above are zero. Therefore, \( \int_{\Omega} \Phi \cdot L\Phi_j \, dx = 0 \).

Since we assumed that \( \Phi_j \) decays to zero exponentially as \( |z| \to \infty \), \( \overline{\Psi}_e \cdot L\Phi_j \) and \( \overline{\Theta}_e \cdot L\Phi_j \) are also integrable on \( \Omega \). Using the same steps above, it can be shown that their integrals are zero. This leads to the second and third equations in system (41).
APPENDIX B

Unlike the case considered in Appendix A, we only know $\Phi_1$ is outgoing as $z \to \pm\infty$. This implies that $\Phi_1$ is bounded at infinity, and we have to consider the integrals on a bounded domain $\Omega_h$ first. To derive Eq. (50), we note that $L\Psi_e = 0$. Therefore,

$$\int_{\Omega_h} \overline{\Psi}_e \cdot L\Phi_1 d\mathbf{x} = \int_{\Omega_h} (\overline{\Psi}_e \cdot L\Phi_1 - \Phi_1 \cdot \overline{\nabla}\overline{\Psi}_e) d\mathbf{x}.$$ 

Using vector identities (59) and (60) and Gauss’ Law, we obtain

$$\int_{\Omega_h} \overline{\Psi}_e \cdot L\Phi_1 d\mathbf{x} = \int_{\partial\Omega_h} \left[ (\nabla \times \Phi_1) \times \overline{\Psi}_e - (\nabla \times \overline{\Psi}_e) \times \Phi_1 + i(b \times \Phi_1) \times \overline{\Psi}_e + i(b \times \overline{\Psi}_e) \times \Phi_1 \right] \cdot d\mathbf{S}.$$ 

Since $\Phi_1$ and $\overline{\Psi}_e$ are periodic in the $x$ and $y$ directions, the integral on the surface parallel to the $z$-axis is zero. Thus

$$\int_{\Omega_h} \overline{\Psi}_e \cdot L\Phi_1 d\mathbf{x} = \int_{D_{xy}} e_3 \cdot \left[ (\nabla \times \Phi_1) \times \overline{\Psi}_e - (\nabla \times \overline{\Psi}_e) \times \Phi_1 + i(b \times \Phi_1) \times \overline{\Psi}_e + i(b \times \overline{\Psi}_e) \times \Phi_1 \right]^{z=h}_{z=-h} dr,$$

where $r = (x, y), D_{xy} = \{(x, y) : |x| < L/2, |y| < L/2\}$, and $e_3 = (0, 0, 1)$ is the unit vector along the $z$-axis. Based in the asymptotic formulae (14) and (49), it is not difficult to show that

$$\lim_{h \to +\infty} \int_{\Omega_h} \overline{\Psi}_e \cdot L\Phi_1 d\mathbf{x} = -2i\gamma L^2 \left(c^+ \cdot d^+ + c^- \cdot d^-\right).$$

Noting that $c^- \cdot d^- = c^+ \cdot d^+$, we obtain Eq. (51).

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