Universal coupled theory for metamaterial bound states in the continuum

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Keywords: metamaterial, bound states in the continuum, coupled-mode theory

Abstract

In this paper, we present a novel universal coupled theory for metamaterial bound states in the continuum (BIC) or quasi-bound states in the continuum (quasi-BIC) which provides ultra-high Q resonance for metamaterial devices. Our theory analytically calculates the coupling of two bright modes with phase information. Our method has much more accuracy for ultra-strong coupling comparing with the previous theories (the coupling of one bright mode and one dark mode and the two bright-mode coupling). Therefore, our theory is much more suitable for BIC or quasi-BIC and we can accurately predict the transmission spectrum of metamaterial BIC or quasi-BIC for the first time.

1. Introduction

Bound states in the continuum (BIC) is initially proposed in quantum mechanics [1], which trapped or guided modes with their frequencies in the frequency intervals of radiation modes [2]. Most recently, BIC has already been introduced for optical systems for the high-resonant phenomenon, such as photonic crystals [3–8], plasmonic structures [9], optical waveguide coupler [10–12], Bragg gratings [13, 14] and metamaterial [15–19, 25]. There are many practical applications for photonic systems, such as lasers [26, 27], sensors [28, 29], high-sensitive medical devices [30, 31], filters [32] and non-linear signal enhanced [33].

The BIC phenomenon can vastly increase the Q-value resonance, especially for the metamaterial, due to the high loss of a single metamaterial structure. The BIC comes from the substantial coupling between the two adjacent single metamaterial structures. Two uniform metamaterial structures have the same frequency and phase of lossy electromagnetic waves, and the lossy waves of two metamaterials have strong interference between each other. Therefore, two lossy electromagnetic waves interfere destructively, which produces the infinite Q-value resonance in the theoretical. In the practical metamaterial, two lossy electromagnetic waves can not be the same due to fabrication. Thus, we can not fabricate infinite Q-value resonance for the metamaterial. However, it can still provide a very high Q value for the metamaterial device, and can widely be used in various applications.

Due to this widely practical BIC metamaterial application, the theory to understand BIC metamaterial is increasingly essential. Currently, there are few different theories to discuss the BIC in the photonic system, such as topological theory [34, 35], Fano resonance theory [36, 37], temporal coupled-mode theory (TCMT) [10–12], the multi-poles theory [33] and coupled theory [19, 20]. However, those theories have their shortcomings. The topological theory employs the topology to explain where the infinite Q-value comes from, but it can not predict how much Q-value is. Fano resonance theory can predict the Q-value, whereas it requires a fitting number q (Fano asymmetry parameter) which is not a physical and fundamental parameter for the metamaterial. TCMT comes from the two coupled mode of waveguides...
system, and the parameters of TCMT is not essential parameters for the metamaterial. Thus, TCMT is more suitable for the optical system. The multi-poles theory [33] is accuracy, but the calculations of the theory is complex, not straightforward for metamaterial BIC.

Recently, a remarkable paper [19] employs the fundamental coupled theory for metamaterial to predict the Q-valve. However, they use the same idea for electrical impedance tomography, which only considers coupling between one bright mode and one dark mode. Moreover, the two bright modes coupling without phase has proposed for metamaterial BIC [20], but their theory do not include the phase information.

When the coupling increasingly strong, the phase difference of two metamaterial structures becomes more and more significant. It brings the big issue which only works for low Q-valve situations because when the two metamaterial structures become identical and phase difference becomes zero, the Q-value is increasingly larger and the external EM field excites two metamaterial structures. Thus, two metamaterial structures become two bright modes and the previously coupled theory [19] is not valid anymore. Furthermore, the phase difference also becomes very important to very high Q-value scenario, where the coupling of two bright mode without phase information [20] start to fail. The coupled theory is very fundamental theory and it widely used in many systems [21–24].

This paper proposes a brand universal coupled theory for metamaterial BIC, which contains the coupling between two bright modes with phase. Therefore, our theory can predict a very high Q-valve situation and the parameters of our view come from the fundamental physical parameters of metamaterial, such as the resonance frequency \( \omega_1, \omega_2 \) for each single metamaterial structure, the loss \( \gamma_1, \gamma_2 \) for each single metamaterial structure and the phase \( \phi_1, \phi_2 \) with each resonance frequency for each single metamaterial structure. The coupling strength \( g \) comes from the physical configuration of two metamaterial structures.

The beauty of our theory is that the resonance frequencies, the loss and the phases are obtained by the spectrum of each signal metamaterial structure, and coupling strength describes the connection of two metamaterial structures.

To demonstrate our theory, we employ two different types of BIC, such as coupling between two cut wires (CWs) [38] (see figure 1(a)) and two split ring resonators (SRRs) [19] (see figure 1(b)). We predict the frequency of BIC and Q-value from the spectrum of transmission THz wave, as shown in figure 1(c).

2. Universal coupled theory

In this section, we present a brand universal coupled theory to describe the BIC in the metamaterial. The idea of our theory comes from the spectrum of transmission THz wave, which is the linear superposition of the transmission spectrum of each metamaterial structure. The linear superposition has a very close relationship with energies in each metamaterial structure. We take the \( |a|^2 \) and \( |b|^2 \) as the energies in each metamaterial structure. Furthermore, the energies in each metamaterial structure can be well described by coupled theory. Besides, the phases of each metamaterial structure become increasingly important for strong coupling and BIC. Thus, we should introduce the phase information into the coupled theory. Finally, we obtain our universal coupled theory as following,

\[
\begin{bmatrix}
\omega - \omega_1 - i\gamma_1 \\
\Omega \\
\omega - \omega_2 - i\gamma_2
\end{bmatrix}
\begin{bmatrix}
a \\
b
\end{bmatrix}
= \begin{bmatrix}
\sqrt{\gamma_1} E \\
\sqrt{\gamma_2} e^{i\phi} E
\end{bmatrix},
\]

where \( \omega \) is the frequency of input THz wave, \( \omega_1, \omega_2 \) represent the frequencies of the metamaterial structures, which is the same as resonant frequency of corresponding metamaterial structure, \( \omega_1 = \omega_1; \omega_2 = \omega_2 \). \( \Omega \) is the coupling strength with loss, due to the loss of transferring energy from one metamaterial structure to another, with \( \Omega = g - i\sqrt{\gamma_1}\gamma_2 e^{i\phi} \), where \( g \) is the coupling strength between two
metamaterial structures. $\gamma_a$ and $\gamma_b$ are the loss terms of metamaterial structures, which is closely to $\gamma_1$, $\gamma_2$ for each single metamaterial structure ($\gamma_a = \gamma_1$; $\gamma_b = (\gamma_1 - \gamma_2)/2$). $\phi$ is the phase information, which can be calculated by the phase $\phi_1$ and $\phi_2$ for each metamaterial structure ($\phi = (\phi_1 - \phi_2)d$, where $d$ is the width of metamaterial structure). $E$ is the amplitude of external exciting THz wave.

Subsequently, we can obtain the energy amplitudes $a$, $b$ of each metamaterial structure by solving the equation (1), as shown,

$$a = \frac{((w - w_b - i\gamma_b)\sqrt{\gamma_a} - \Omega\sqrt{\gamma_b}e^{i\phi_a})E}{(w - w_b - i\gamma_b)(w - w_a - i\gamma_a) - \Omega^2},$$ (2)

$$b = \frac{((w - w_a - i\gamma_a)\sqrt{\gamma_b} - \Omega\sqrt{\gamma_a}e^{i\phi_b})E}{(w - w_b - i\gamma_b)(w - w_a - i\gamma_a) - \Omega^2}. (3)$$

Then we calculate the effective susceptibility which is the linear superposition with energy amplitudes $|a|^2$ and $|b|^2$. The effective electric susceptibility of the metamaterial can be written as [39]

$$\chi_{\text{eff}} = \frac{\sqrt{\gamma_a}a + \sqrt{\gamma_b}b}{\epsilon_0E}. (4)$$

Finally, we obtain the transmission spectrum with $T \approx 1 - \text{Im}(\chi_{\text{eff}}) [19]$, as shown,

$$T \approx 1 - \text{Im} \left( \frac{(w - w_a - i\gamma_a)\gamma_b e^{i\phi_a} + ((w - w_b - i\gamma_b)\gamma_a - 2\Omega\sqrt{\gamma_a}e^{i\phi_a})}{(w - w_b - i\gamma_b)(w - w_a - i\gamma_a) - \Omega^2} \right). (5)$$

3. Examples

Firstly, we present the BIC with coupling between two CWs (as shown in figure 1(a)) and we can obtain the resonance frequency ($\omega_1$, $\omega_2$), the loss ($\gamma_1$, $\gamma_2$) and phase with each resonance frequency ($\phi_1$, $\phi_2$) for each single metamaterial structure, as shown in figure 2. We use the full-wave simulations of each metamaterial structure and put them together for BIC to get the corresponding transmission spectrum (see the black line of figure 3).

Figure 2. Full-wave simulations of (a) transmission spectrum of single left CW structure, (b) transmission spectrum of single right CW structure, (c) the phase of single left CW structure and (d) the phase of single right CW structure.
Figure 3. The black line is the full-wave simulations of CWs BIC (see the smaller figure) and our predict the transmission spectrum of CWs BIC by employing our theory, as shown in red line.

Figure 4. Full-wave simulations of (a) transmission spectrum of single left SRR structure, (b) transmission spectrum of single right SRR structure, (c) the phase of single left SRR structure and (d) the phase of single right SRR structure.

From the results, we can obtain the resonance frequency $\omega_1 = 0.256 \text{ THz}$, $\omega_2 = 0.248 \text{ THz}$, the loss $\gamma_1 = 0.028 \text{ THz}$, $\gamma_2 = 0.03 \text{ THz}$ and phase with each resonance frequency $\phi_1 = 0.297$, $\phi_2 = 0.31$ for each single metamaterial structure. Therefore, $\omega_a = 0.256 \text{ THz}$, $\omega_b = 0.248 \text{ THz}$, $\gamma_a = 0.028 \text{ THz}$, $\gamma_b = -0.004 \text{ THz}$ and $\phi = 2.3$. From the result of BIC (as shown in black line of figure 3), we observe the BIC phenomenon with Fano resonance transmission spectrum with $Q = w_{\text{BIC}}/\Delta w = 160$, where $\Delta w$ is the full width at half maximum of Fano resonance.

Due to complex analytic calculation of coupling strength $g$ between two metamaterial structures, we employ the fitting calculation by applying our universal coupled theory (equation (4)) to obtain the coupling strength $g$, as shown in the red line of figure 3. As we can see that the transmission spectrum of
Figure 5. The black line is the full-wave simulations of SRRs BIC (see the smaller figure) and our predict the transmission spectrum of SRRs by employing our theory, as shown in red line.

our theory (equation (4)) is consistent with the full-wave simulation of CWs BIC. Therefore, our theory can not only well describe and explain BIC for metamaterial but also can predict the frequency and Q-value of BIC.

In order to demonstrate the universality of our theory for different coupled metamaterial structures, we verify our theory by using coupling between two SRR as BIC as shown in figure 1(b). We take the same steps above where get the full-wave simulations of each single SRR (see figure 4) and BIC (see figure 1(b)) to obtain the corresponding transmission spectrum (the spectrum of each single structure see figure 4 and the spectrum of BIC shows black line of figure 5). As we can see from figure 4, $\omega_a = \omega_1 = 0.573 \text{THz}$, $\omega_b = \omega_2 = 0.636 \text{THz}$, $\gamma_a = \gamma_1 = 0.144 \text{THz}$, $\gamma_b = (\gamma_1 - \gamma_2)/2 = -0.008 \text{THz}$, $\phi = (\phi_1 - \phi_2)d = 2.1$ and the transmission spectrum of two SRRs BIC with $Q = 18$. Subsequently, we employ our universal coupled theory (equation (4)) with those parameters by fitting coupling strength $g$ to calculate the transmission spectrum for BIC, as shown in red line in figure 5. It is easy to find that our method is very closely to full-wave simulations of two SRRs BIC. In other words, our universal coupled theory is valid for BIC with different types of metamaterial structures.

4. Discussion

Our method proposes the two bright modes coupling with phase information and employs it into the BIC metamaterial. Therefore, our theory can easily predict the transmission spectrum of BIC and much more suitable for high Q resonance cases comparing with previous researches [19, 20]. In order to demonstrate the superiority of our theory, we employ full-wave simulations of low Q, medium Q and high Q cases for CW BIC (figure 1(a)) and SRR BIC (figure 1(b)), respectively, as shown in the black lines of figure 6. Subsequently, we apply the coupling of one bright mode and one dark mode [19], two bright modes coupling without phase information [20] and our theory to fit the full-wave simulations of low Q, medium Q and high Q cases respectively. The blue lines demonstrate the fitting results of the coupling of one bright mode and one dark mode [19], and green lines illustrate the fitting results of the two bright modes coupling without phase information [20], and the red lines show the fitting results of our theory in figure 6.

From the results of figure 6, we can easily obtain that the fitting results of the previous theories and our theory can both well predict the low Q case of the transmission spectrum of BIC, as shown in figures 6(a) and (e). When the Q-value continuously increases, the fitting results of previous researches [19, 20] start to have some errors in the medium Q cases, as shown in the blue lines and green lines in figures 6(b) and (f). When the high Q-value cases for BIC (see figures 6(c) and (g)) occurs, the previous theory of the coupling of one bright mode and one dark mode [19] can not be valid anymore and the previous theory can not give the Fano spectrum of BIC at all. The reason for this phenomenon is that when the two metamaterial structures become increasingly uniform ($\Delta l$ turns smaller and smaller), the Q-value of BIC becomes larger and larger. When the high Q cases occur, two metamaterial structures can be excited by the input THz wave. Thus, the two metamaterial structures turn into two bright modes and the theory of one bright mode and dark mode can not be valid anymore. When the very-high Q cases for BIC (as shown in figures 6(d) and
Figure 6. The black lines, blue lines, green lines and red lines demonstrate the full-wave simulations, the fitting results of previous theory [19], the fitting results of two bright modes without phase information [20] and the fitting results of our theory, respectively. The (a), (b), (c) and (d) represent the low-$Q$, medium $Q$, high $Q$ and very high $Q$ cases for CW BIC (see figure 1(a)). The (e), (f), (g) and (h) show the low-$Q$, medium $Q$ and high $Q$ cases for SRR BIC (see figure 1(b)).
(h)), the two bright modes coupling without phase information [20] fails to predict the Fano spectrum of BIC. Even two bright modes coupling [20] has already considered two metamaterial structure becoming two bright modes, but the phase difference of two metamaterial structures has significant effect on the coupling. To sum up, the fitting results of our theory have good performance of fitting results to predict BIC for low Q, medium Q, high Q and very high Q cases, as shown in red lines of figure 6. Therefore, our theory surpasses and contains the previous theory [19, 20], especially for high Q-value resonance BIC.

5. Conclusion

In this paper, we propose a new theory to describe metamaterial BIC by employing the coupling theory of two bright modes with phase information. Our new theory can universally explain metamaterial BIC and very accurately predict the frequency of BIC and Q-value of resonance, even for the very high Q case.

Acknowledgments

This work acknowledges funding from National Key Research and Development Program of China (2019YFB2203901); National Science and Technology Major Project (Grant No.: 2017ZX02101007-003); National Natural Science Foundation of China (Grant Nos.: 61565004; 61965005; 61975038; 62005059). The Science and Technology Program of Guangxi Province (Grant No.: 2018AD19058). Innovation Project of GUET Graduate Education(2021YCXS129). WH acknowledges funding from Guangxi oversea 100 talent project; WZ acknowledges funding from Guangxi distinguished expert project.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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