Passive nonreciprocal transmission and optical bistability based on polarization-independent bound states in the continuum

1 Introduction

The control of light flow in modern optical devices relies significantly on nonreciprocal transmission [1–5]. However, the manufacture of nonreciprocal electromagnetic devices on traditional platforms is challenging due to the symmetric time-invariant and linear permittivity and permeability tensors. Thus, three physical mechanisms can break reciprocity. Firstly, the application of a dc magnetic bias to magneto-optical materials can obtain the asymmetric permittivity tensor leading to light isolation. Secondly, the time-variant properties of some materials can achieve optical nonreciprocity. Finally, strong electromagnetic nonlinear effects can break reciprocity in different settings, such as using the harmonic generation [6], using phase transitions in VO₂ layer [7], and nonreciprocal optical nonlinear metasurfaces [8]. Nonlinearity has attractive features and does not require any external bias, making it a promising approach for integration with traditional optical platforms. As light passes through mirror asymmetric devices in opposite directions, the different refractive indices caused by nonlinear materials affects the transmission efficiency of light differently, breaking the reciprocity property. Nonreciprocal transmission by nonlinear metasurfaces methods is based on the Kerr effect, which depends on the local strength of the electric field. Nonreciprocal methods based on nonlinearity have been applied in various systems due to their simplicity and applicability. However, since nonlinear materials typically have weaker optical nonlinearities, these self-biased devices must rely on high-\(Q\) optical resonance [9].

Bound states in the continuum (BICs) are a unique phenomenon within the continuous spectrum of extended states, exhibiting perfect localization in space and infinite theoretical lifetimes [10–16]. Initially proposed in 1929 by Neumann and Wigner as an electronic system in the context of quantum mechanics, the problem remained a mathematical curiosity for nearly five decades without experimental
evidence to support its existence. But now, such interesting, novel, and essential phenomena have been proposed in various wave systems, such as mechanics, electronics, acoustics, and optics. In the field of nanophotonic, the state of optical BIC has been widely discussed over the past few decades due to its high $Q$ factor strong resonance. To this day, BICs have been demonstrated to construct in various mechanisms, including symmetry mismatch, parameter tuning, environment engineering, topological charge evolution, parity-time symmetry, and so on. In addition to the well-known symmetry-protected BICs (SP-BICs) developed by the symmetry-restricted out-coupling \cite{17–22}, the existence of optical BIC modes can also be classified as the accidental BIC or Fredrich–Wintergen (FW-BIC) \cite{23–25}\ in brief.

In this letter, we present a novel approach to achieve nonreciprocal transmission using a nonlinear method. We demonstrate that this can be accomplished through the utilization of polarization-independent resonances that are governed by SP-BIC in a metasurface with $C_{4v}$ symmetry \cite{26}. Generally, the rotational or mirror symmetry of a structure is broken by in-plane \cite{27–29} and out-of-plane symmetry perturbation \cite{30,31}, making resonances excited by SP-BIC polarization-sensitive. However, we report the exciting discovery of polarization-independent SP-BIC in metasurfaces made of equidistantly spaced perturbed high-refractive-index dielectric disks arrays, which retain $C_{4v}$ features. To further understand the mechanism of resonances, we calculate the scattering powers of different multipoles \cite{32,33}. Ultimately, we show that a nonlinear metasurface with $C_{4v}$ symmetry can facilitate free-space nonreciprocal propagation by breaking reciprocity based on polarization-independent SP-BIC. Our findings pave the way for the design and development of new devices with nonreciprocal transmission properties.

2 Polarization-independent q-BIC

Let us start with a Si metasurface composed of cylindrical meta-atoms with an etched hole; see Figure 1(a). The radii of the cylindrical element atom and the etched cylindrical hole are $R$ and $r$, respectively. And the height of cylindrical meta-atoms and etched cylindrical holes are $H$ and $h$, respectively. Four cylindrical meta-atoms with the same Geometric parameters form a $2 \times 2$ square supercell shown in Figure 1(b). We control the asymmetry of the metasurface by adjusting the position of the etched cylindrical holes. When the etched hole and the cylindrical meta-atoms share the same center, the period of the metasurface is $p = 500$ nm. Then we let this etch hole move along the dotted line towards the center $O$ displayed in Figure 1(c). We define this asymmetric factor $\alpha$ as the distance the etched hole moves toward the center divided by the difference between the radius of the metasurface $R$ and etched cylindrical holes $r$, that is $\Delta d/(R - r)$. When $\alpha \neq 0$, the period of the metasurface changes to $a = 2^*p$. Obviously, no matter how this asymmetric factor changes, our structure remains $C_{4v}$ symmetry.

According to the description above, we set the metasurface depicted in Figure 1(c) with geometry parameters $p = 500$ nm, $R = 150$ nm, $r = 50$ nm, $H = 200$ nm, and $h = 100$ nm. The refractive index of the Si is set as 3.46 \cite{1}, and $\chi (3) = 2.8e^{-18}$ m$^2$/V$^2$. The metasurface is placed in the air with a refractive index of $n = 1$. The finite element method (FEM) is utilized to calculate the linear transmission spectrum by applying periodic conditions in both the $x$ and $y$ directions of the supercell. The dispersion of eigenmodes of the metasurface is shown in Figure 2(a). Since the $C_{4v}$ symmetry of the structure, the BIC mode is polarization independent. The mode we discussed at the $\Gamma$ point has been marked with a red circle. The blue dotted line is a

![Figure 1](image_url): Schematic diagram of the structure. (a) Schematic of the nonreciprocal metasurface: by combining structural asymmetry and material nonlinearity, a monochromatic beam impinging from the up and down sides of the device experiences markedly different transmission levels. (b) Geometry parameters of the supercell consisting of four same square unit. (c) When the etched hole moves towards the center of the circle $O$, the true BIC mode turns to q-BIC mode.
light-line. At the highly symmetric case when $\delta = 0$, the eigenmode’s electric field and magnetic field at $\Gamma$ point are depicted in the inset of Figure 2(a), indicating the existence of BIC modes. Next, we calculated the transmission spectra for different asymmetric factors shown in Figure 2(b). Clearly, for $\alpha = 0$ ($\Delta d = 0$ nm), no transmission dips can be observed, and the linewidth vanishes. As $\alpha$ continues to increase, the linewidth of transmission spectra increases, and the resonant wavelengths have a blueshift. The q-BIC associated with the non-radiative Fano resonance mode is intrinsically accompanied by a giant field concentration in the resonators. Figure 2(c) and (d) illustrate the magnetic field distributions at the peak wavelength (1191.3 nm), (1180.2 nm) identified in Figure 2(a) for the case $\alpha = 0.2$, $\alpha = 0.6$, respectively. The maximum field concentration occurs in the metasurface, a magnetic field enhancement factor larger than 380 is identified within the cylindrical meta-atoms with a hole at $\alpha = 0.2$, and at $\alpha = 0.6$, the magnetic field enhancement factor is about 140. Consistent with the trend of decreasing $Q$-factor upon increasing $\alpha$, the magnetic field enhancement factor showed a significant drop.

3 Multipole analysis of q-BIC

To further figure out the mechanism of the BIC mode, the scattering powers of different multipoles, including the electric dipole (ED), the magnetic dipole (MD), the toroidal dipole (TD), the electric quadrupole (EQ), and the magnetic quadrupole (MQ) in the Cartesian coordinate system were analyzed and demonstrated in Figure 3(a) and (b). As seen in Figure 3(a), the contribution of the TD (deep blue solid line) is predominant, indicating that the BIC mode is mainly induced by the TD. By decomposing the $x$, $y$, and $z$ components of the TD scattering power in Figure 3(b), we find that the $y$ component of the scattering power from the TD dominates the TD scattering power dissipation and is almost equal to it in value. And compared to the $y$ component, the $x$ and $z$ components of the scattered power of the TD are almost close to 0. The distribution of the normalized electromagnetic field for the BIC mode of the metasurface is presented in Figure 3(c) and (d). The black arrow represents the displacement current density and magnetic field vector in Figure 3(c) and (d), respectively. For BIC Mode, as shown in Figure 3(c), circulation orientations of displacement currents in the $y$ direction of the Si neighboring
cylindrical meta-atoms are opposite and the same in the $x$ direction of the neighboring cylindrical meta-atoms, which indicates that the opposite phase magnetic dipoles along the $z$ direction are induced in the $y$ direction meta-atoms pair. Figure 3(d) depicts the magnetic field distribution at the $x-z$ plane. As indicated by the white circle, opposite-phase magnetic dipoles form a closed magnetic vortex in the $x-z$ plane. The magnetic field vector circulates clockwise between adjacent cuboids in the intra-cluster $x$ direction meta-atoms and counterclockwise between adjacent cuboids in the inter-cluster $x$ direction neighboring meta-atoms. The magnetic field distribution is head to tail, which is characteristic of TD multipole.

4 Free space nonreciprocal transmission and Bistability

To implement the nonreciprocal transmission in the proposed polarization-independent metasurface, we further perform nonlinear optical simulations using the FEM method in the frequency domain. In order to achieve optical isolation, the out-of-plane asymmetry is particularly important. We agree that the light from the $+z$ direction to the $-z$ direction is incident in the forward direction (port 1), and the opposite direction is incident in the back direction (port 2). Figure 4(a) shows the transmittance spectra at $\alpha = 0.6$ when illuminated from each port with an incident intensity of 40 MW/cm$^2$. The green line in Figure 4(a) displays the linear response of the structure, with a Fano resonant signature stemming from the superposition of a high-$Q$ resonance in the dielectric atoms and a low-$Q$ background resonance at the air-metasurface interfaces. According to the Kerr nonlinear effect, different field enhancements will lead to different refractive indices and thus give rise to the shift of resonant frequency. Since the resonator is out-of-plane asymmetric, this shift is distinct for excitation from opposite sides, enabling free space nonreciprocal transmission. Figure 4(a) reveals this mechanism by comparing linear and nonlinear responses at the same power from opposite sides.

Next, we consider the calculated nonlinear response of the metasurface, which is the same as Figure 4(a), presented in Figure 4(b)–(d). Figure 4(b)–(d) show the transmittance versus input power for three excitation wavelengths. Analogous to a p-n junction diode, the solid curves in Figure 4(b)–(d) represent effective optical I–V curves for light with a wavelength of $\lambda = 1181$ nm, $\lambda = 1181.5$ nm, $\lambda = 1182$ nm, respectively. For Figure 4(b), in the linear regime, when the incident power is relatively low, light is highly
transmitted on both sides of the metasurface. As the incident power increases to 12 MW/cm², the transmission intensity drops sharply in the backward direction (blue curve) while remaining very high in the forward direction (red curve), and the unidirectional transmission persists until around 17.4 MW/cm². And here, the nonreciprocal intensity range (NRIR) is defined as the ratio of intensities from opposite directions for which transmission experiences a fast transition [1]. In fact, NRIR is closely related to the out-of-plane asymmetry of the structure, while having no relationship with excitation wavelengths. For Figure 4(c) and (d), the simulated intensity-dependent port-to-port transmission for excitation for another two different excitation wavelengths from Figure 4(b) explains the mechanism that NRIR is excitation wavelength independent. For any excitation wavelength and transmission direction, the minimum transmission intensity in the nonlinear response is dependent on the linear transmission spectra (Figure 4(a)), the different transmission intensities are shown in Figure 4(b)–(d) for different excitation wavelengths. The transmittance drops to almost zero with the increasing incident power for Figure 4(b), but as shown in Figure 4(c) and (d), there is no way to get to zero for the minimum transmittance.

In particular, the trade-off for the maximum non-linear forward transmission and the NRIR, can be explained by the temporal coupled mode theory (TCMT). In the context of TCMT, a single resonance with 2 ports is expressed as

\[
\frac{da}{dt} = (-j\omega_0 - \gamma_1 - \gamma_2 - \gamma_v)a + (k_1 \ k_2) \left( \begin{array}{c} s_{1+} \\ s_{2+} \end{array} \right) \left( \begin{array}{c} s_{1-} \\ s_{2-} \end{array} \right),
\]

\[
C = \left( \begin{array}{cc} r_B & -jB \\ -jB & r_B \end{array} \right) \left( \begin{array}{c} s_{1+} \\ s_{2+} \end{array} \right) + (k_1 \ k_2) \left( \begin{array}{c} s_{1-} \\ s_{2-} \end{array} \right),
\]

Here, \( a \) is the resonance amplitude, \( \omega_0 \) is the resonance frequency, \( \gamma_v \) is the intrinsic cavity loss rate and \( \gamma_v = 0 \) since we do not consider losses at this point, \( \gamma_{in} = \gamma_1 + \gamma_2 \) is the cavity decay rate due to coupling into the two ports, with decay rates \( \gamma_1 \) and \( \gamma_2 \), respectively, \( s_{1+} \) and \( s_{2+} \) are the amplitudes of the incoming waves from the two ports, \( s_{1-} \) and \( s_{2-} \) are the amplitudes of the outgoing waves, and \( k_1, k_2 \) are the complex coupling coefficients between the ports and the resonance. The scattering matrix \( C \) represents the
direct coupling between incoming and outgoing waves, with 
$r_B$ and $t_B$ being the corresponding amplitude reflection and 
transmission coefficients, which satisfy $r_B^2 + t_B^2 = 1$.

According to the energy conservation and time-reversal 
symmetry property of the cavity, the conditions can be 
obtained as follows,

$$k_1 = \sqrt{2\gamma_1 e^{i\beta_1}}, \quad k_2 = \sqrt{2\gamma_2 e^{i\beta_2}}. \tag{2}$$

$$\begin{pmatrix} r_B & i t_B \\ i t_B & r_B \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = - \begin{pmatrix} k_1 \\ k_2 \end{pmatrix}. \tag{3}$$

Through the temporal coupled mode theory and the con-
ditions, the transmission coefficient of the system can be 
derived easily as

$$T = |k| = a \left( x \mp x_0 \right)^2 / (x^2 + 1). \tag{4}$$

Here, $x = (\omega_0 - \omega)\gamma$ is the detuning factor of the resonator, and 
$x_0 = \left[ 4\omega_0^2 - 1 \right] / \left[ |\gamma_0(e^{i\gamma_0})|^2 \right]$ is a characteristic parameter of 
the resonator that provides the detuning from the reso-
nance frequency at which transmission is zero. The positive (negative) sign in Eq. (3) corresponds to the case where the 
frequency of the transmission zero is higher (lower) than the resonant frequency. If we define $\kappa = |k_1|^2 / |k_2|^2 = \gamma_1 / \gamma_2$ as the asymmetry factor from different ports, Eq. (3) can be 
rewritten as

$$T = \frac{4\kappa}{(\kappa + 1)^2} \left( x \mp x_0 \right)^2 / \left( x^2 + 1 \right) \left( x_0^2 + 1 \right). \tag{5}$$

Considering that for a symmetric Fano resonator max-
imum transmission is unitary, we know that asymmetry 
requires the following bound on the transmission of Fano 
resonators when the resonator is symmetric, $\kappa = 1$:

$$T \leq \frac{4\kappa}{(\kappa + 1)^2}. \tag{6}$$

It can be shown that the NRIR is always equal to the 
linear electromagnetic asymmetry, $NRIR = \kappa = |E_1|^2 / |E_2|^2$, 
thus,

$$T_{\text{max}}^{\text{nonlinear}} = \frac{\kappa}{\kappa + 1}. \tag{7}$$

Therefore, although increasing the out-of-plane asym-
metry of the structure can obtain an immense NRIR value, 
the cost is lower in transmission intensity.

Next, we describe the mechanism of nonlinear bistabi-
lity. If we assume the resonators to be nonlinear, the nonlinear-
earity results in a shift of the resonance frequency of the resonator as

$$\omega_0 = \omega_{0,\text{lin}} \left( 1 - \frac{|a|^2}{|a_0|^2} \right). \tag{8}$$

where $\omega_{0,\text{lin}}$ is the resonance frequency in the linear regime and $|a_0|^2$ is the energy in the nonlinear cavity. Considering 
that the nonlinear isolator is excited from the $i_{th}$ port 
with a monochromatic signal $s_{i_+}$ at frequency $\omega_0$, we get the 
equation as follows,

$$\left( 1 - \frac{\omega_0}{\omega_{0,\text{lin}}} \right) \left[ \left( \omega - \omega_0 \right)^2 + \gamma^2 \right] = \frac{|k|^2 p_{in}}{|a_0|^2}. \tag{9}$$

Here, $p_{in} = |s_{i_+}|^2$, $\gamma$ and $k_i$ are the same as in the linear 
regime, $\omega_0$ is the input intensity.

From this equation, we can understand an important 
mechanism in nonlinear optical cavities. For different input 
light intensities, there will be different resonance frequency 
ofsets and the overall response of Fano nonlinear isolators 
can be adjusted by the factor $\kappa = |k_1|^2 / |k_2|^2$ for different 
incident ports. So that the NRIR of nonreciprocal response 
could be largely tuned and the bistability phenomenon can 
be obtained.

Therefore, although increasing the out-of-plane asym-
metry of the structure can obtain an immense NRIR value, 
the cost is lower in transmission intensity.

According to the discussion in the previous article, we 
will again analyze the influence of in-plane asymmetry and 
out-plane asymmetry on nonreciprocal transmission. The 
in-plane asymmetry is usually utilized to transform the true 
BICs to q-BICs since true BICs possess an infinite Q-factor, 
zero linewidth, and cannot be excited. We can adjust the 
degree of in-plane asymmetry $a$ to tune the $Q$-factor of the 
metasurface and maximize the nonlinear interactions, 
but it is not necessary to achieve nonreciprocity. Instead, 
the out-plane asymmetry is vital for nonreciprocal behavior 
along the $+z$ and $-z$ directions. By controlling the height $H$ 
and $h$, we can adjust the electromagnetic asymmetry of the 
structure and the value of NRIR.

Next, we keep other parameters unchanged and adjust 
the height of the cylindrical meta-atoms $H$ and the height 
of the etch cylindrical hole $h$ to confirm the effect of out-of-
plane asymmetry on NRIR. The intensity-dependent trans-
mission of three representative metasurfaces is shown in 
Figure 5(a–c) with out-of-plane asymmetries ranging from 
values $(H = 500 \text{ nm}, h = 100 \text{ nm},$ Figure 5(a), $H = 500 \text{ nm},$ 
h = 80 nm, Figure 5(b), and $H = 500 \text{ nm},$ h = 50 nm, 
Figure 5(c)). In each panel, the insets show the linear trans-
mittance spectra and a vast field enhancement of the electro-
mechanical field, respectively. As anticipated, the device with 
the most enormous out-of-plane asymmetry (Figure 5(c), $H = 500 \text{ nm}, h = 50 \text{ nm}$) also features the broadest nonreciprocal 
intensity range (NRIR = 2.2), while its maximum transmis-
sion in the forward direction is limited to $\sim 0.7$. Strong
field enhancement can result in nonreciprocal transmission at lower power, while different out-of-plane asymmetries will lead to different transmission levels and NRIR. Consistent with the previous, the minimum and maximum transmission obtained in the nonlinear response match the minimum and maximum transmission in the corresponding linear transmission spectrum. When we reduce the out-of-plane asymmetry, the corresponding forward maximum transmission efficiency will increase, while the NRIR shrinks.

We obtain the intensity-dependent transmission while sweeping the power up (blue curve) and down (green curve) at $H = 200$ nm, $h = 100$ nm, shown in Figure 6(a), and calculate the wavelength-dependent transmission with the wavelength scanned from short to long wavelength and then also from long wavelength to short shown in Figure 6(b). For Figure 6(a), because of the existence of third-order nonlinearity, the bistable phenomenon can be predicted. There will be two stable states in the case of the same incident power. For power up, the transmission efficiency suffers a sudden drop at an intensity of about $I_{\text{peak}} = 17$ MW/cm$^2$ with increasing intensities, corresponding to the transition from the one stable state, which has a high transmittance, to another one which has low transmittance. Then as the incident power gradually decreases from high power, the system remains in the stable state, which is transmitted with less efficiency until the peak intensity is about $I_{\text{peak}} = 12$ MW/cm$^2$, after which it jumps back to another steady state which is transmitted with more efficiency. For Figure 6(b), we scan the transmittance with increasing wavelength (red curve) and decreasing wavelength (blue curve), respectively. Since the initial field condition of

Figure 5: Nonlinear characterization with different values of $H$, $h$: (a) $H = 500$ nm, $h = 100$ nm, (b) $H = 500$ nm, $h = 80$ nm, (c) $H = 500$ nm, $h = 50$ nm. In each panel, the insets above show linear transmission spectra of three devices, the insets below display the electric field enhancement.

Figure 6: Optical bistability. (a) Measured the forward transmission of the metasurface by scanning the power up (blue curve) and down (cyan curve). (b) Measured the forward transmission of the metasurface by scanning with increasing wavelength (blue curve) and decreasing wavelength (red curve).
different wavelengths, the various Kerr shifts take place in different ways of scanning wavelengths. All nonlinear simulations in the above were performed with a wavelength-increasing scan.

5 Conclusions

In conclusion, we present the design and analysis of a polarization-independent nonreciprocal metasurface with C$_{4v}$ symmetry, based on symmetry-protected BIC resonances. The Q-factor and linewidth of q-BICs were adjusted by manipulating the distance between the etched hole and the center O of the metasurface. Our investigation revealed that the toroidal dipole was the main contributor to the mechanism of symmetry-protected BIC mode. We observed that the scattering power from the y component of the toroidal dipole was dominant. Exploiting the nonlinear properties of the material in combination with the out-of-plane asymmetry of the metasurface structure, we achieved free space nonreciprocal transmission. Our study also highlights the ability to tune the nonreciprocal intensity range by controlling the structure parameters. We discuss the trade-off between the maximum nonlinear forward transmission and the nonreciprocal intensity range. Additionally, we observe the bistable phenomena of the nonreciprocal system. Our research demonstrates a robust and widely applicable approach for obtaining free-space fully-passive nonreciprocal propagation by leveraging q-BICs and material nonlinearities. Our findings pave the way for various applications, including the protection of high-power lasers and nonreciprocal signal routing for analog and quantum computing.

Acknowledgments: Yuanjiang Xiang was partly sponsored by China Ministry of Education under National Natural Science Foundation of China (Grant Nos. 61875133 and 11874269); Natural Science Foundation of Hunan Province (Grant Nos. 2021JJ30135 and 2021JJ30149).

Research funding: National Natural Science Foundation of China (Grant Nos. 61875133 and 11874269); Natural Science Foundation of Hunan Province (Grant Nos. 2021JJ30135 and 2021JJ30149); Chongqing Natural Science Foundation (CSTB2022NSCQ-MSX0872).

Author contribution: Shiwen Chen, and Yixuan Zeng initiated the idea. Shiwen Chen performed the theoretical analysis and discussed the results. All authors contributed to writing the paper.

Conflict of interest: The authors declare no conflicts of interest regarding this article.

Informed consent: Informed consent was obtained from all individuals included in this study.

Data availability: The datasets generated and/or analysed during the current study are available from the corresponding author upon reasonable request.

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