Extreme Diffraction Control in Metagratings Leveraging Bound States in the Continuum and Exceptional Points

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Coupled resonances in non-Hermitian systems can lead to exotic optical features, such as bound states in the continuum (BICs) and exceptional points (EPs), which have been recently emerged as powerful tools to control the propagation and scattering of light. Yet, similar tools to control diffraction and engineer spatial wavefronts have remained elusive. Here, it is shown that, by operating a metagrating around BICs and EPs, it is possible to achieve an extreme degree of control over coupling to different diffraction orders. Sub-wavelength metallic slit arrays stacked on a metal-insulator-metal waveguide, enabling a careful control of the coupling between localized and guided modes are explored. By tuning the coupling strength from weak to strong, the overall spectral response can be tailored and the emergence of singular features, like BICs and EPs can be enabled. Perfect unitary diffraction efficiency with large spectrum selectivity is achieved around these singular features, with promising applications for selective wavefront shaping, filtering, and sensing.

1. Introduction

Metasurfaces can manipulate light propagation at will based on arrays of tailored subwavelength inclusions.[1–3] Since they typically operate within the far-field radiation continuum, they are inherently a non-Hermitian (open) platform. Their dispersion and spectral features can be engineered to support bound states in continuum (BICs)[4–6] and exceptional points (EPs).[7–9] BICs are self-sustained eigenmodes embedded within the radiation continuum, typically manifested by a vanishing linewidth as we continuously vary a parameter associated with the structure symmetry[10–13] or the coupling strength between multiple modes or resonance channels.[14–19] The associated high-Q resonances around a BIC have been widely employed to construct ultra-sharp transmission and reflection spectra, leading to performance-enhanced applications, such as BIC lasing[20,21] and sensing.[22] The non-Hermitian nature of metasurfaces enables also the emergence of EPs, which are branch point singularities in the $k$-vector space of the metasurface at which multiple eigen-frequencies and the corresponding eigenmodes coalesce.[23–25] Such singularities offer potential opportunities for enhanced sensitivity, due to their super-linear dependence to small perturbations.[26–28] Currently, both BICs and EPs in metasurfaces have been mostly focused on the manipulation of the spectral/temporal properties of the impinging optical signals, namely, to control the zeroth diffraction-order transmission/reflection features for incident plane waves.[10–13,23–25]

In parallel, few-diffraction-order (FDO) metagratings, capable of suppressing undesired diffraction orders and redirecting the incident power to preferred directions with unitary efficiency, have been developed for efficient and extreme wavefront engineering with less spatial resolution demand when compared with conventional phase-gradient metasurfaces.[41,42] In this paper, we introduce a platform to control the emergence of BICs and EPs near the Brillouin edge of an FDO metagrating, tailoring the diffraction spectra in extreme ways. Specifically, we show how, by continuously tuning the coupling strength between localized and guided resonant modes, we can map the dispersion relation onto the trajectory of perfect diffraction towards the $−1$st order. Our work connects BICs and EPs with light diffraction, offering novel opportunities for nanophotonic engineering, such as embedded wavefront shaping and spatial wavefront sensing.[43–46]

2. Results and Discussion

The geometry of interest is shown in Figure 1a, and it is composed of a layer of subwavelength metallic slits with thickness $t$,
1st or −1st diffraction orders are within the light cone, as shown by the green patches in Figure S1a,b in the Supporting Information. At the LM or GM resonances, the −1st diffraction efficiency in reflection approaches unity, while specular reflection is suppressed, leading to a peak in $R_0$, and a dip in $R_1$ at the trajectory of the LM or GM dispersion curves (Figure S2, Supporting Information). By simultaneously combining LM and GM resonances in the FDO regime of a metagrating (inset of Figure 1a), the coupling between LM and GM offers rich opportunities to engineer the overall scattering response involving multiple diffraction channels.

Generally, the subwavelength slits in our metagrating operate as a periodic perturbation for the waveguide modes in the underlying dielectric region, leading to avoided crossing between forward and backward GMs. The coupling strength can be readily tuned by the LM resonance in the gap area, which is controlled by the slit layer thickness $t$. When the LM resonance frequency coincides with the crossing point of the forward/backward GMs ($t = 0.425\lambda$), maximum coupling is achieved (Figure 1b). In this strong coupling scenario, a large Rabi splitting between the GMs (higher and lower quadratic bands) can be observed. Between the quadratic bands, a flat band emerges associated with the LM, with a vanishing linewidth at the Brillouin boundary ($k_x = \pi/p$), corresponding to a BIC. The dispersion of coupled GMs and LMs is reflected into the dip and peak trajectories of the specular reflection coefficient $R_{\pm}$ (left panel of Figure 1b) and −1st diffraction $R_{1}$ (right panel of Figure 1b), respectively, offering a flexible way to manipulate light diffraction and wavefront shaping based on high-Q BICs.

In contrast, when the LM resonance is tuned far away from the forward/backward GM crossing point at $t = 0.201\lambda$ (Figure 1c), the coupling strength reaches its minimum, and the forward/backward GMs get close together. In this regime, due to the weak coupling between the structure and the background environment, the linewidths of both the $R_{\pm}$ dip and $R_1$, peak trajectories become much smaller. As shown in the following, both BIC and EPs arise near the crossing area of the forward/backward GMs in this weak coupling scenario.

Figure 2a shows the corresponding band structure (eigen-frequency $\text{Re}(k_x)$ vs parallel wavevector $k_x$) in the weak coupling regime, for the same parameters as in Figure 1c. The coupled GMs are highlighted by red and blue curves, consistent with the dip/peak trajectories of the $R_{\pm}$ spectra in Figure 1c. Remarkably, by zooming close to the crossing points, we find a degenerate line around $k_x = \pi/p$, as shown in Figure 2b. Since the metagrating is an open system, the imaginary part of the eigen-frequency is generally nonzero within the light cone, leading to a finite radiative $Q$-factor of the GM leaky modes. Figure 2c shows the radiative $Q$-factor dispersion of the coupled GM, corresponding to the modes indicated by the same color in Figure 2b. At the Brillouin boundary $k_x = \pi/p$, although $\text{Re}(k_x)$ of the two modes is degenerate, their $Q$-factors (or $\text{Im}(k_x)$) are largely different. One mode (mode 1) has a lower $Q$-factor, while the other (mode 3) has a diverging $Q$-factor, corresponding to a BIC. In addition, the $Q$-factors become degenerate when $|k_x - \pi/p|$ exceeds the threshold value 0.012$\pi/p$, at which both $\text{Re}(k_x)$ and $Q$-factor ($\text{Im}(k_x)$) are degenerate (mode 2), implying the emergence of EPs within this diffractive regime. Figure 2d–f shows field patterns for eigenmodes 1–3. For modes 1 and 2 (EP mode), the GM field

![Figure 1. a) Schematic of our metagrating geometry, composed of a metallic subwavelength slit array with period $p$, slit width $w$, and thickness $d$, and a metallic substrate. Localized (LM) and guided (GM) modes emerge in the metallic slit and dielectric spacer layer, respectively, providing a powerful way to manipulate and control the diffraction orders $R_0$ and $R_{-1}$, within the few-diffraction-order regime, as denoted by the green area of the dispersion diagram in the inset. b) Diffraction efficiency of the 0th (left panels) and 1st (right panels) orders as we vary the parallel wavevector $k_x$ for different slit layer thicknesses: $t = 0.425\lambda$ corresponding to strong coupling and $t = 0.201\lambda$ corresponding to weak coupling. The metal is treated here as a perfect electric conductor (PEC), which is a good approximation for metal at terahertz and microwave frequencies. Both the wavevectors $k_0$, $k_x$ are normalized to $2\pi/p$. BIC is formed at the wavelength specified by $k_0 = 2\pi/\lambda_0 = 2\pi/p$, and the incident angle $\theta_b = 30^\circ$ ($k_0 = k_0\sin\theta_b$) at the Brillouin boundary $k_x = 0.5(2\pi/p)$.](image-url)

![Figure 2. a) Corresponding band structure (eigen-frequency $\text{Re}(k_x)$ vs parallel wavevector $k_x$) in the weak coupling regime, for the same parameters as in Figure 1c. The coupled GMs are highlighted by red and blue curves, consistent with the dip/peak trajectories of the $R_{\pm}$ spectra in Figure 1c. Remarkably, by zooming close to the crossing points, we find a degenerate line around $k_x = \pi/p$, as shown in Figure 2b. Since the metagrating is an open system, the imaginary part of the eigen-frequency is generally nonzero within the light cone, leading to a finite radiative $Q$-factor of the GM leaky modes.](image-url)
penetrates the slit area (convex field distribution), and some fields leak into the background. In contrast, mode 3 (BIC mode) is characterized by fields strictly confined in the dielectric slab layer, with a null just below the slit area, forming a concave field distribution. There is no radiation to the upper semi-space, reflecting the bound nature of the mode, despite supporting a transverse momentum compatible with radiation.

Figure 3 shows the evolution of the modes as we continuously change the coupling strength. By varying the slit layer thickness, the localized gap mode bridging energy to the background environment and the guided modes is tuned, leading to different coupling strengths between forward and backward GMs. The resonance wavelength of the localized mode can be roughly predicted by the Fabry–Perot (FP) condition, \( m \frac{\lambda_0}{2n_{\text{eff}}} = t \), where the integer \( m \) is the mode index and \( n_{\text{eff}} \) is the effective index of the subwavelength slit waveguide. When the slit layer thickness \( t \) is tuned such that \( \lambda_0 \) coincides with the GM eigen-frequency at the Brillouin boundary (cases II, IV, VI in Figure 3a, b), the strong interaction between the gap LMs, the forward, and backward GMs gives rise to an avoided crossing with maximum Rabi splitting. The corresponding field patterns (Figure 3c) show that the eigenmodes are strongly coupled, and become hybrids of the gap LM (field concentrated in the slit area) and GM (field concentrated in the dielectric layer). In addition, we always find one mode with field totally confined in the dielectric layer vanishing below the slit (concave mode), due to the destructive interference of LMs and GMs. Although such concave mode lies above the light line and thus within the FDO regime, it does not sustain radiation, corresponding to a BIC in the diffractive regime.

For other values of \( t \), for which the LM resonance frequency deviates from the GM at the Brillouin boundary, the mutual coupling strength between forward and backward GMs decreases, leading to reduced Rabi splitting, while the BIC arises either on the upper or lower quadratic band (Figure S3, Supporting Information). In particular, if \( t \) is chosen such that \( (m + 1/2) \frac{\lambda_0}{2n_{\text{eff}}} = t \), and \( \lambda_0 \) is the GM eigen-frequency at the Brillouin boundary (cases I, III, V), then the GM is located in the middle between two adjacent ordered LMs, representing the largest separation between GMs and LMs. In this situation, the coupling strength is minimum, with zero Rabi splitting with respect to the real part of eigen-frequency \( \text{Re}(k_0) \). At the same time, the imaginary part of the eigen-frequency \( \text{Im}(k_0) \) splits at this point, with one mode yielding zero (BIC state) and the other one yielding a finite radiation loss (Figure S4, Supporting Information).

Multiple diffraction orders of the metagrating support radiative loss channels, resulting in a non-Hermitian system. For the minimum coupling (I, III, V) scenario, the LM eigen-frequencies

Figure 2. Band diagram and field patterns of eigenmodes in the anticrossing region, with same parameters as in Figure 1c. a) Band diagram of the real part of \( k_0 \) versus \( k_x \) and its b) zoomed region near the crossing point. c) Radiative quality (\( Q \)) factor. d–f) Field patterns (\( H_z \)) of 1) lowest \( Q \)-factor radiative mode, 2) EP mode, and 3) BIC mode as indicated in (c).
Figure 3. Evolution of mode coupling by varying the slit layer thickness. a) Upper panel: eigen-frequencies, middle panel: Rabi splitting, and lower panel: radiative Q-factor evolution with slit layer thickness \( t \). b) 1st diffraction efficiency spectra with varying parallel wavevector \( k_x \) and total wavevector \( k_0 \), for higher-order weak coupling cases with III) \( t = 0.698 \) p, IV) \( t = 1.194 \) p, and strong coupling cases with slit layer thickness IV) \( t = 0.946 \) p, VI) \( t = 1.442 \) p, respectively. The other parameters are \( w = 0.05 \) p, \( d = 0.1 \) p fixed. c) Field patterns corresponding to the modes indicated in each band of (b).

Figure 4. Embedded wavefront shaping. a) Field patterns \((H_z)\) demonstrating wavefront deflection of a Gaussian beam incident on a periodic metagrating (with parameters \( w = 0.05 \) p, \( t = 0.425 \) p, \( d = 0.1 \) p) tuned at the quasi-BIC resonance (middle panel) and a little detuned from the quasi-BIC resonance (upper and lower panels), the operating frequencies are \( k_0 = 0.952, 1.006, 1.1 \) (in unit of \( 2\pi/p \)), the incident angles are 24.85°, 23.43°, and 21.32° (with fixed \( k_x = 0.4 \)), and the reflection angles are 24.85°, −36.61°, and 21.32°, respectively. The simulation domain is of size 51 p × 16 p. b) Field patterns \((H_z)\) demonstrating wavefront focusing of a Gaussian beam incident on a modulated metagrating (with parameters \( w = 0.2 \) p, \( t = 0.425 \) p, \( d = 0.1 \) p) with quadratic phase profile at the quasi-BIC resonance (middle panel). When the wavelengths are slightly shifted from the quasi-BIC frequency, a focusing phenomenon in the abnormal reflection direction is replaced by specular reflections (upper and lower panels). The operating frequencies are \( k_0 = 0.95, 1.07, 1.15 \), the incident angles are 24.90°, 21.95°, and 20.35° (with fixed \( k_x = 0.4 \)), respectively, and the reflection angles are 24.90°, −34.11°, 20.35°, respectively. The simulation domain has the size of 750 p × 375 p.
are far away from the GMs, and the effective Hamiltonian of the system can be written as coupled GM resonances between forward and backward modes

$$H_{\text{eff}} = \begin{pmatrix}
\omega_0 & v_g \left(k_x - \frac{\pi}{p}\right) \\
v_g \left|k_x - \frac{\pi}{p}\right| & \omega_0 - iv_d
\end{pmatrix}$$

for which the complex eigenvalues are

$$\omega_{\pm} = \omega_0 - \frac{v_g}{2} \pm \nu_g \sqrt{\left|k_x - \frac{\pi}{p}\right|^2 - \left(\frac{v_g}{2v_0}\right)^2}$$

here, $v_g$ is the group velocity, $v_d$ is the radiative loss rate difference between convex and concave GMs. This expression indicates that EPs arise at

$$k_x = \frac{\pi}{p} \pm \frac{v_g}{2v_0}$$

which ensures that the complex eigen-frequencies become degenerate. This condition is slightly away from the Brillouin boundary $k_x = \pi/p$, as numerically confirmed in the band diagrams of both Re$(k_x)$ and Im$(k_x)$ in Figure S4 in the Supporting Information. We note that, the BICs and EPs associated with the evolution of strong coupling and weak coupling have been discussed in other optical systems,[47–49] while our present study deals with the coupling of guided Bloch modes of similar decay rates, where the weak coupling mediated by a localized mode is sufficient for creating EPs.

We can use our metagrating platform, supporting tailored BICs and/or EPs in the diffractive regime, to demonstrate sensitive wavefront shaping applications embedded in a continuous broadband spectrum. Figure 4a shows how these features can be used for anomalous reflection. Near the BIC resonance (middle panel of Figure 4a), anomalous reflection occurs due to near-unity ~1st diffraction. However, when the working frequency $k_x$ slightly deviates from the resonance condition, the impinging beam undergoes ordinary specular reflection, as shown in the upper and lower panels of Figure 4a. The frequency difference is so small that we are not able to distinguish the different wavelengths between the anomalous and ordinary reflection scenarios from the field patterns. Figure 4b shows wavefront focusing using a quadratic phase modulation across the aperture.[50–52] Only at resonance the impinging beam can be focused at the ~1st diffraction order (middle panel of Figure 4b), while at other slightly detuned frequencies the impinging beam undergoes normal specular reflection (upper and lower panels of Figure 4b).

3. Conclusion

In conclusion, here we demonstrated perfect diffraction metagratings supporting tailored BICs and EPs. By continuously tuning the coupling between the supported LMs and forward/backward GMs in the FDO regime through the slit layer thickness, we observed continuous Rabi splitting evolution between coupled modes, and obtained dative BICs at the Brillouin boundary, as well as two dative EPs. The bands supporting BICs and EPs correspond to the peak trajectory of the ~1st diffraction efficiency spectra, providing a direct link between the emergence of BICs and EPs and the diffraction response of the underlying metagratings. With the sharp spectral features of the BIC, the metagratings offer exciting opportunities for novel spectrum-sensitive diffraction and wavefront shaping applications. Leveraging EPs in the diffractive regime, robust wavefront phase modulation with topological features can be envisaged.[53] Our findings may find interesting implications for embedded wavefront shaping and sensing applications.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (NSFC) (Grants 62075084), the National Key Research and Development Program of China (2021YFB2802003), the Guangdong Provincial Innovation and Entrepreneurship Project (Grant 2016ZT06D0081), the Guangdong Basic and Applied Basic Research Foundation (2020A1515010615), the Guangzhou Science and Technology Program (202102020566), the Simons Foundation and the Air Force Office of Scientific Research MURI program.

Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

bound states in the continuum, exceptional points, metagrating

Received: October 28, 2021
Revised: January 26, 2022
Published online: March 6, 2022

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