Fourier-component-engineered metasurfaces support continuous bound states in the continuum and Dirac cone dispersions

Sun-Goo Lee, Seong-Han Kim, and Chul-Sik Kee
Integrated Optics Laboratory, Advanced Photonics Research Institute, GIST, Gwangju 61005, South Korea
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Conventional photonic lattices, including metamaterials and photonic crystals, exhibit various interesting physical properties due to the periodic modulations in lattice parameters. Here, we introduce new types of photonic lattices, namely Fourier-component-engineered metasurfaces, that do not possess the first-order Fourier harmonic component in the periodically modulated lattice parameters, and demonstrate that the metasurfaces support the continuous bound states in the continuum and Dirac cone dispersions near the second stop bands. The concept of engineering Fourier harmonic components in periodic modulations provides a new method to manipulate electromagnetic waves in artificial periodic structures.

Subwavelength photonic lattices with thin-film geometries, such as metasurfaces \cite{1,2} and photonic crystal slabs \cite{4,5}, have attracted significant attention in recent years owing to their substantial abilities of manipulating electromagnetic waves. Unlike the usual thin homogeneous dielectric layers that are governed by the Fresnel equations and Snell’s law \cite{3}, photonic lattices can capture the incident light resonantly through the lateral Bloch modes and reemit the light with predesigned electromagnetic responses \cite{7}. By appropriately designing the individual constituents in the lattices, several interesting physical effects and useful applications, which cannot be achieved with conventional dielectric materials, can be realized in an extremely compact format even as a single-layer film \cite{8,10}.

Recently, the bound states in the continuum (BICs) and Dirac cone dispersions in planar photonic lattices have been studied extensively. BICs are unusual electromagnetic eigenstates that remain well localized in open photonic systems even though they can coexist with the continuous spectrum of outgoing waves \cite{11,12}. BICs are associated with various fascinating physical phenomena such as the sharp Fano resonances \cite{13}, enhanced nonlinear effects \cite{14}, and topological nature \cite{15,16}. Dirac cone dispersion refers to the closed band state with cross-over at a discrete specific incident angle. Small variations in high-frequency photonic lattices \cite{25,26}. However, the BICs in artificial periodic structures.

Different types of BICs have been studied in versatile planar photonic lattices \cite{25,26}. However, the BICs introduced in the literatures thus far are strongly sensitive to the wavevector of Bloch modes in the lattices. Hence, high-Q Fano resonances due to the BICs can be obtained at a discrete specific incident angle. Small variations in the incident angle significantly reduce the resonance $Q$ factor in the spectral responses. In this letter, we introduce new types of photonic lattices, called Fourier-component-engineered (FCE) metasurfaces, that do not possess the first-order Fourier harmonic component, and demonstrate that the metasurfaces support continuous BICs in a wide range of wavevectors instead of a specific discrete wavevector. Here, we treat Dirac cones with BICs because the Dirac cones in the vicinity of the $\Gamma$ point can be accompanied with BICs in planar photonic lattices \cite{27}. With the out-of-plane radiation loss, the Bloch modes exhibit anomalies in the dispersion curves, such as leaky-band flattening and exceptional points, that ruin the Dirac cone dispersion \cite{31,32}.

FCE metasurfaces proposed herein are based on the fact that in the vicinity of the second stop band, radiation loss is caused by the first-order Fourier harmonic component. Figures \ref{fig:1}(a) and \ref{fig:1}(b) illustrate two of the simplest representative one-dimensional (1D) photonic lattices, i.e., binary dielectric grating (BDG) and zero-contrast grating (ZCG), that support BICs. The periodic modulations in the dielectric constant of BDGs and the variations in thickness of ZCGs generate photonic band gaps at the Bragg condition $k_z = qK/2$, as shown in Fig. \ref{fig:1}(c), where $k_z$ is the Bloch wavevector, $K = 2\pi/\Lambda$ is the magnitude of the grating vector, and $q$ is an integer representing the Bragg order. In this study, we focus on the second band gap ($q = 2$) of the fundamental TE$_0$ mode because BICs and Dirac cones are associated with the second stop bands in many cases. As conceptually illustrated in Fig. \ref{fig:1}(d), the second leaky stop band is formed primarily by the direct coupling $h_2$ with $|\Delta k_z| = 2K$ between two counter propagating waves $\sim \exp(\pm ikz)$, and secondarily by the radiative coupling $h_1$ with $|\Delta k_z| = K$ between the guided and radiating waves \cite{33}.

The coupling processes illustrated in Fig. \ref{fig:1}(d) can be clarified by solving the 1D wave equation given by \cite{34}:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right) E_y(x, z) + \epsilon(x, z)k_0^2 E_y(x, z) = 0,$$  \hspace{1cm} (1)

where $k_0$ denotes the wave number in free space. Equation (1) can be solved by expanding the periodic dielectric function $\epsilon(x, z)$ in a Fourier series and the electric field $E_y$ as a Bloch form \cite{32}. For the 1D lattice BDG shown...
where \( \Omega_0 \) stop band and \( \Omega_0 \) is the Bragg frequency under vanishing index modulation, and the coupling coefficients are given by

\[
h_0 = \Omega \int_{-\infty}^{\infty} \epsilon_0(x) \varphi(x) \varphi^*(x) dx,
\]

\[
h_1 = \frac{K^3 \Omega^4 \xi_0}{8} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x, x') \varphi(x') \varphi^*(x) dx' dx,
\]

\[
h_2 = \frac{K^2 \Delta \varepsilon}{4} \int_{-\infty}^{\infty} \varphi(x) \varphi^*(x) dx,
\]

where \( G(x, x') \) denotes the Green’s function for the diffracted field. The dispersion relation in Eq. (2) can be obtained numerically by calculating the coupling coefficients in Eqs. (3)–(5), appropriately describes the second stop band of weakly to moderately modulated photonic lattices. Because the coupling coefficients \( h_1 \) and \( h_2 \) are formed by the first and second Fourier harmonics, respectively, we can interpret that the second stop band is formed by the interplay between two coupling processes, as illustrated in Fig. (d).

Equation (2) indicates that the leaky stop band with two band edges \( \Omega^a = \Omega_0 + h_2/(K\hbar) \) and \( \Omega^b = \Omega_0 - (h_2 + i2\hbar t)/(K\hbar) \) opens at \( k_z = 0 \). The symmetry-protected BIC appears with the purely real eigenfrequency \( \Omega^a \) without \( h_1 \) at the band edge when the spatial electric field distribution is an asymmetric cosine function \( A = -B \). More, the topologically-protected BICs can be found at the generic \( k \) points when the real part of \( h_1 \) is zero. A small variation in the lattice parameters moves the position of the topologically-protected BIC along the dispersion curves because \( \text{Re}(h_1) \) becomes zero at a slightly different \( k \) point with different lattice parameters. The symmetry- and topologically-protected BICs have been studied in several cases in various planar photonic structures. Inspired by the fact that the eigenfrequencies in Eq. (2) become purely real without the contribution of the first-order Fourier harmonic \( \epsilon_1 \cos(Kz) \), in this study, we investigate BICs and Dirac cones in the FCE metasurfaces, which do not possess the first-order Fourier harmonic component, that correspond to the representative BDG and ZCG shown in Figs. (a) and (b), respectively, through the finite element method (FEM) simulations.

In Fig. (b) we first compare the key properties of the conventional BDG and those of the corresponding FCE metasurface. As shown in Fig. (b), the FCE metasurface has complex dielectric functions \( \epsilon_a - \epsilon_1 \cos(Kz) \) and \( \epsilon_b - \epsilon_1 \cos(Kz) \) when \( |z| < \rho A/2 \) and \( |z| \geq \rho A/2 \), respectively, while the conventional BDG has simple step-like dielectric functions with \( \epsilon_a \) and \( \epsilon_b \) in the high and low dielectric constant parts, respectively. Figure (b) demonstrates that the second band gap opens at \( k_z = 0 \) for both the BDG and FCE metasurface and the symmetry-protected BICs appear at the upper band edges. However, the spatial electric field \( (E_y) \) distributions in the insets in Fig. (b) show that the lower edge mode with the symmetric field distribution in the conventional lattice is radiative out of the lattice, while the lower edge mode in the FCE metasurface is appropriately localized in the lattice. The reduction in the out-of-plane radiation in the FCE metasurface can be observed by investigating the \( Q \) factors of the Bloch modes plotted in Fig. (c). In the conventional BDG, the symmetry-protected BIC in the upper band exhibits a \( Q \) factor that is larger than \( 10^5 \) at the \( \Gamma \) point but the \( Q \) values decrease abruptly and approach to the value of \( Q \) factor of leaky modes (\( \sim 10^3 \)) in the lower band as \( k_z \) moves away from the \( \Gamma \) point. In the FCE metasurface, the symmetry-protected BIC exhibits a \( Q \) factor that is larger than \( 10^5 \) and the \( Q \) values decrease as \( k_z \) moves away from the \( \Gamma \) point. However, the Bloch modes in both the upper and lower band branches have high \( Q \) values (\( \sim 10^8 \)) in the computational range of \( |k_z| \leq 0.12 \) K. The \( Q \) factors in the FCE metasurface are approximately \( 10^5 \) times larger than those in the BDG with the same lattice parameters.
further, the resonance line width by the upper band mode are observed in the transmittance curve. As by the upper and lower band Bloch modes, respectively, the spatial electric field (second stop band. Insets with blue and red colors illustrate the quasi-BICs with finite high-Q resonance line width. In diverse practical applications, such as t, Δε, and ρ, they could find useful applications to overcome the discrete nature of the BICs in conventional photonic lattices.

Dirac cone dispersions with closed band states, Re(Ωa) = Re(Ωb), can be achieved by adjusting the lattice parameters ρ and/or Δε [31]. Figure 3(a) shows the evolution of the band edge frequencies Re(Ωa) and Re(Ωb) for the conventional BDG and FCE metasurface as a function of ρ. As ρ increases from zero, the band gap opens and its size |Re(Ωa) − Re(Ωb)| first increases, then decreases, and finally becomes zero when ρ = ρc. The band gap reopens and its size first increases, then decreases, and finally approaches zero when ρ is further increased and approaches 1. At the closed band state with ρ = ρc, as shown in Fig. 3(b), the dispersion curves of the conventional BDG exhibit a finite range of Bloch wave vectors Δkz, where ∂ΩRe/∂kz ≈ 0. In contrast, the dispersion curves of the FCE metasurface cross as straight lines, and ∂ΩRe/∂kz ≠ 0 at kz = 0 at the closed band state. The leaky band flattening in the DBG shown in Fig. 3(b) is evident from the analytical dispersion relations in Eq. (2), which can be rewritten as

\[
Ω(k_z) = Ω_0 - \left( i h_1 ± \sqrt{k_z^2 - Re(h_1)^2} \right) / (K h_0) \tag{6}
\]

at the closed band state with h2 = Im(h1). Equation 6 reveals that leaky band flattening occurs ow-

except the profile of the dielectric function.

The symmetry-protected BICs are perfectly embedded eigenvalues with an infinite Q factor and varnishering resonance line width. In diverse practical applications, quasi-BICs with finite high Q values and narrow spectral responses are favorable. Figure 2(d) illustrates the transmission spectra through the BDG and FCE photonic lattices as a function of incident angle θ. At normal incidence with θ = 0°, the BDG structure only exhibits the low-Q resonance by the lower band edge mode. The embedded BIC in the upper band edge mode is not shown in the transmittance curve. When θ = 1°, both the high-Q resonance (quasi-BIC) and low-Q resonance by the upper and lower band Bloch modes, respectively, are observed in the transmittance curve. As θ increases further, the resonance line width by the upper band mode increases rapidly and becomes close to that by the lower band mode. Two low-Q resonances are observed in the spectral response when θ = 7°. The transmittance curve through the FCE metasurface does not show the embedded BIC in the upper band when θ = 0°. However, the resonance line width by the lower band mode is extremely narrow, unlike the case of conventional BDG. As θ increases from zero, two quasi-BICs by the lower and upper band modes are observed and the resonance line widths remain narrow when θ = 7°. Because the continuous quasi-BICs always exist in the vicinity of the second stop bands of the FCE metasurface irrespective of lattice parameters such as t, Δε, and ρ, they could find useful applications to overcome the discrete nature of the BICs in conventional photonic lattices.

![Figure 2](image2.png)

**FIG. 2.** Comparison between the conventional photonic lattice and FCE metasurface. (a) Dielectric functions as a function of z. (b) FEM simulated dispersion relations near the second stop band. Insets with blue and red colors illustrate the spatial electric field (Ez) distributions of the band edge modes at the y = 0 plane. Vertical dotted lines represent the mirror planes in the computational cells. (c) Calculated radiative Q factors of the upper and lower bands. (d) Evolution of transmission spectra vs the incident angle ϑ. In the FEM simulations, we use the structural parameters ϵavg = 4.00, Δε = 1.00, ϵs = 1.00, t = 0.50 Λ, and ρ = 0.40.
FIG. 4. Simulated dispersion relations (a) and Q factors (b) near the second stop band of the ZCG structure and FCE metasurface. (c) Simulated band edges for the conventional ZCG with ρ = 0.60, tavg = 0.50 Λ, tc = tavg + (1 − ρ)Δt, cs = 4.00, and ϵs = 1.00. (d) Dispersion relations at the closed band state for the conventional ZCG with ρc = 0.44910 and for the FCE metasurface with ρc = 0.52128.

they depict the Q factors of the Bloch modes in the upper and lower bands as a function of kz. In the conventional ZCG, the symmetry-protected BIC in the lower band exhibits a Q factor larger than 10^{15} at the Γ point, but the Q value decreases abruptly and approach the value of the Q factor (∼ 10^9) of leaky modes in the upper band as kz moves away from the Γ point. In the FCE metasurface, the symmetry-protected BIC exhibits a Q factor larger than 10^{15} and the Q value decreases as kz moves away from the Γ point. However, the Bloch modes in both the upper and lower bands have high Q values, larger than ∼ 10^{9}, in the computational range of |kz| ≤ 0.12 Λ. The Q factors in the FCE metasurface are approximately 10^{4} times larger than those in the ZCG with the same lattice parameters except the thickness profile. Figure 4(c) shows that the closed band states with Re(Ωc) = Re(Ωt) can be achieved by adjusting the lattice parameter ρ for both the ZCG structure and FCE metasurface. At the closed band state with ρ = ρc, as revealed in Fig. 4(d), the FCE metasurface exhibits the Dirac cone dispersion with ∂ΩRe/∂kz ≠ 0 at kz = 0, while the ZCG demonstrates the flat dispersion curves near kz = 0.

In conclusion, we introduced the concept of FCE metasurfaces that do not possess the first-order Fourier harmonic component in the periodically modulated lattice parameters, such as the dielectric constant and thickness, and demonstrated that the new types of lattices support the continuous quasi-BICs and Dirac cone dispersions near the second stop bands. Because the out-of-plane radiation is primarily due to the first-order Fourier harmonic component of the periodic modulation in lattice parameters, the Bloch modes of the FCE metasurface possess high radiative Q factors and there is no leaky band flattening and exceptional point near the second stop bands. Our study is limited to the simplest 1D lattices associated with the first-order Fourier harmonic component. However, the extension of this work to higher-order Fourier harmonics and 2D lattices is feasible.

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* sungoolee@gmail.com
  csklee@gist.ac.kr

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