Guided modes of an open periodic waveguide, with a periodicity in the main propagation direction, are Bloch modes confined around the waveguide core with no radiation loss in the transverse directions. Some guided modes can have a complex propagation constant, i.e., a complex Bloch wavenumber, even when the periodic waveguide is lossless (no absorption loss). These so-called complex modes are physical solutions that can be excited by incident waves whenever the waveguide has discontinuities and defects. We show that the complex modes in an open dielectric periodic waveguide form bands, and the endpoints of the bands can be classified to a small number of cases, including extrema on dispersion curves of the regular guided modes, bound states in the continuum, degenerate complex modes, and special diffraction solutions with blazing properties. Our study provides an improved theoretical understanding on periodic waveguides and a useful guidance to their practical applications.

Complex modes in an open lossless periodic waveguide

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Guided modes of an open optical waveguide, by definition, are confined around the waveguide core [1]. Without absorption and radiation losses, the propagation constant of a guided mode is normally a real number. For lossless two-dimensional (2D) waveguides (with 1D refractive index profiles) that are invariant along the waveguide axis, it can be proved that the propagation constant of any guided mode is real. Leaky modes and evanescent modes in the continuous spectrum have complex propagation constants, but they are not guided modes, since their fields are not confined around the core. However, it is known that open lossless 3D waveguides (with 2D refractive index profiles) can support full-vector guided modes with complex propagation constants [2, 3].

For closed waveguides, these so-called complex modes are known since the 1960’s [4]. The existence of complex modes is related to the fact that the full-vector eigenvalue problem at a fixed frequency with the propagation constant being the eigenvalue is non-Hermitian. While the complex modes do not carry power along the waveguide axis, they are physical solutions that can be excited by incident waves for waveguides with discontinuities or defects, and they cannot be ignored in any rigorous waveguide analysis when eigenmode expansions are used. It is also known that the complex modes are the cause for numerical instability of the full-vector paraxial beam propagation method, a classical modeling technique for wave propagation in optical waveguides [2, 3].

In this Letter, we show that complex modes also exist in 2D open lossless periodic waveguides for which the refractive index varies periodically along the main propagation direction (i.e., the waveguide axis). To the best of our knowledge, a systematic study of complex modes in open periodic waveguides is currently not available. Our results indicate that complex modes form bands, and for each band, the propagation constant is a complex-valued function of the real frequency. We also analyze the endpoints of complex-mode bands. It is shown that the solution at an endpoint can be a regular guided mode with a real propagation constant, a bound state in the continuum (BIC) [3, 11], a degenerate complex mode, or a diffraction solution with special blazing properties [12]. In the following, we present theoretical and numerical results for complex modes of a 2D periodic waveguide.

We consider a lossless 2D structure that is invariant in $x$, periodic in $y$ with period $L$, and surrounded by vacuum for $|z| > d$. A special example is a periodic array of circular cylinders surrounded by vacuum as shown in Fig. 1. The cylinders are parallel to the $x$ axis and periodically arranged along the $y$ axis. The radius and dielectric constant of the cylinders are $a$ and $\varepsilon_c$, respectively, and we can let $d = L/2$. If incident waves are specified in the surrounding homogeneous media, the periodic structure serves as a diffractive element, but for waves propagating in the $y$ direction, it can be regarded as a 2D periodic waveguide. For simplicity, we consider time-harmonic waves in the $E$ polarization. Thus, the $x$ component of the electric field, denoted as $u$, satisfies the following Helmholtz equation

$$\partial^2_y u + \partial^2_z u + k^2 \varepsilon(r) u = 0, \quad (1)$$

where $k$ is the freespace wavenumber, $r = (y, z)$, and $\varepsilon(r)$ is the real dielectric function.

An eigenmode of the periodic waveguide is given by $u(r) = e^{i\beta y} \phi(r)$, where $\beta$ is the propagation constant (or Bloch wavenumber) and $\phi$ is periodic in $y$ with period $L$. For a real frequency (i.e., a real $k$), if $\phi(r) \to 0$ exponentially as $z \to \pm \infty$, the eigenmode is a guided mode. A

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{A periodic array of circular cylinders surrounded by vacuum.}
\end{figure}
differential equation for $\phi(r)$ can be easily derived by inserting the Bloch form into Eq. (1). This equation for $\phi$, the periodic condition in $y$, and the boundary condition for $z \rightarrow \pm \infty$, give rise to an eigenvalue problem defined on domain $\Omega = \{(y, z) : |y| < L/2, |z| < \infty\}$ (one periodic of the structure), where $\beta$ is the eigenvalue and $k$ is a real parameter. This eigenvalue problem for guided modes is non-Hermitian.

The leaky modes are solutions of a slightly different eigenvalue problem with an outgoing radiation condition for $z \rightarrow \pm \infty$. If the periodic structure is regarded as a diffractive element, it is useful to regard $\beta$ as a real parameter, $k$ as the eigenvalue, and impose outgoing radiation condition as $z \rightarrow \pm \infty$. This leads to a different non-Hermitian eigenvalue problem with complex-frequency outgoing radiating solutions, i.e., the resonant modes (also known as resonant states, guided resonances, or quasi-normal modes) [13, 14]. It is also useful to consider the eigenvalue problem for which $k$ is the (possibly complex) eigenvalue and $\beta$ is related to $k$ such that $\beta/k$ is real and given [15].

For a lossless periodic waveguide, guided modes with a real $\beta$ typically exist below the light line, i.e., for $k < |\beta|$, and $\beta$ can be restricted to the interval $(-\pi/L, \pi/L)$ due to the periodicity. Such a guided mode will be referred to as a regular guided mode in this Letter. For $|z| > d$, the wave field of a regular guided mode can be expanded in evanescent plane waves as

$$u(r) = \sum_{m=\infty}^{\infty} c_m^\pm e^{i\beta_m y + \gamma_m (d+z)}, \quad |z| > d,$$  \hspace{1cm} (2)

where $\beta_0 = \beta$, $\beta_m = \beta + 2\pi m/L$, and $\gamma_m = \sqrt{\beta_m^2 - k^2}$ for each integer $m$. Some guided modes with a real $\beta$ can exist above the light line, i.e., for $k > |\beta|$, and they are the BICs [13, 14]. Equation (2) is still valid for a BIC, but $c_m^\pm$ must be zero, if the corresponding $\gamma_m$ is pure imaginary (for $m = 0$ and possibly other integers). We are concerned with complex modes, i.e., guided modes with a complex $\beta$. Although there is no absorption loss ($\varepsilon$ is real) and no radiation loss ($\phi \rightarrow 0$ as $z \rightarrow \pm \infty$), the propagation constant $\beta$ of a complex mode has a nonzero imaginary part. If the standard complex square root function (with a branch cut along the negative real axis) is used to define $\gamma_m$, Eq. (2) remains valid for complex modes.

Let $u(r)$ be a complex mode with a propagation constant $\beta = \beta' + i\beta''$, where $\beta' = \text{Re}(\beta)$ and $\beta'' = \text{Im}(\beta)$ are the real and imaginary parts of $\beta$, and $\beta'' \neq 0$. By reciprocity, we have another complex mode $v(r)$ with propagation constant $-\beta$. Since $k$ and $\varepsilon(r)$ are real, $\overline{\beta}$ and $\overline{\gamma}$ (the complex conjugates of $u$ and $v$), satisfy the same Helmholtz equation and are also complex modes. The propagation constants for $\overline{u}$ and $\overline{v}$ are $-\overline{\beta}$ and $\overline{\gamma}$, respectively. Therefore, if $0 < \beta' < \pi/L$, we have four related complex modes $\{u, \beta\}, \{v, -\beta\}, \{\overline{u}, -\overline{\beta}\}$ and $\{\overline{v}, \overline{\beta}\}$. If $\beta' = 0$, there are only two distinct propagation constants $\pm i\beta''$. Typically, the corresponding complex modes are non-degenerate, then $P$ must be proportional to $u$. With a proper scaling, we can force $u$ to be a real function. Similarly, $v$ can also be scaled as a real function. The case for $\beta' = \pi/L$ is similar. It is necessary to regard $\beta = \pi/L + i\beta''$ and $-\overline{\beta} = -\pi/L + i\beta''$ as the same propagation constant. If the corresponding complex modes are non-degenerate, we can scale $u$ and $v$ as real functions.

Like the regular guided modes, the complex modes form bands. But since $\beta$ is complex and $k$ is real, it is more convenient to regard $\beta$ as a complex-valued function of $k$. Each complex-mode band corresponds to an interval of $k$ in which $\beta$ is a differentiable function of $k$. Multiplying Eq. (1) by the reciprocal mode $v$, and integrating on $\Omega$, we can easily derive the following formula

$$\frac{d\beta}{dk} = \frac{k}{\int_{\Omega} \varepsilon(r) uv dr} \left( \frac{\partial u}{\partial y} \right).$$ \hspace{1cm} (3)

For the special cases with $\beta' = 0$ or $\beta' = \pi/L$, we know that $u(r)$ and $v(r)$ can be scaled as real functions, thus $d\beta/dk$ is a pure imaginary number. This means that there could be complex-mode bands with fixed $\beta' = 0$ or $\beta' = \pi/L$.

The power carried by a guided mode is proportional to

$$P(u) = \int_{-\infty}^{\infty} \text{Im} \left( \frac{\partial u}{\partial y} \right) dz,$$ \hspace{1cm} (4)

and it is a constant independent of $y$. For any complex mode, we have $P(u) = 0$. This can be easily proved by multiplying $\overline{u}$ to Eq. (1), integrating on $\Omega$, and considering the imaginary part. In addition, for a complex mode, $-i\int_{\Omega} \overline{u} \partial_y u d\Omega = L P(u) = 0$. For a regular guided mode, we can assume $v = \overline{u}$, but for a complex mode, $v \neq \overline{u}$, and thus, $\int_{\Omega} v \partial_y u d\Omega$ is not proportional to $P(u)$ and is typically nonzero.

To gain a better understanding on the complex modes, we analyze the conditions for the endpoints of the bands. Let $k_\ast$ be the freespace wavenumber at the end of a complex-mode band, then as $k \rightarrow k_\ast$, we have $u \rightarrow u_\ast$ and $\beta \rightarrow \beta_\ast$. Assuming $0 \leq \text{Re}(\beta_\ast) \leq \pi/L$, the endpoints may be classified as follows.

1. $\beta_\ast$ is real and $k_\ast < \beta_\ast$ (below the light line). It is clear that $u_\ast$ has to be a regular guided mode. Meanwhile, the propagation constant of $\overline{u}$ (complex conjugate of the reciprocal mode) is $\overline{\beta}$ and it also tends to $\beta_\ast$. If the guided mode with freespace wavenumber $k_\ast$ and propagation constant $\beta_\ast$ is non-degenerate, then the limit of $\overline{u}$ is also $u_\ast$ (up to a constant), i.e., two complex modes $u$ and $\overline{u}$ collapse to one regular guided mode. In such case, $\int_{\Omega} v \partial_y u d\Omega = 0$, and $\beta$ (as a function of $k$) has an
infinite slope at $k_\ast$. As we shall see in the numerical examples below, this type of endpoints may appear for both $\beta_\ast < \pi/L$ and $\beta_\ast = \pi/L$.

2. $\beta_\ast$ is real and $\beta_\ast \leq k_\ast < 2\pi/L - \beta_\ast$ (above the light line with one opening radiation channel). In this case, the zeroth diffraction channel is open, that is, the $m = 0$ terms in Eq. (4) are propagating plane waves. If $\beta^\ast$ associated with $u(r)$ is positive, then $\gamma_0 \to i\delta_0$ for $\delta_0 = (k_\ast^2 - \beta^2)^{1/2} > 0$ as $k \to k_\ast$; thus, the $m = 0$ terms in Eq. (4) are incoming plane waves. Since it is impossible to sustain a bounded solution with incoming waves only, we must have $c_0^r = c_0^i = 0$. Therefore, the limit solution $u_\ast$ must be a BIC. Assuming the BIC is non-degenerate, then the two complex modes $u$ and $\tau$ collapse to the same BIC, $\int_\Omega v_\ast \partial_y u_\ast \, dr = 0$, and $d\beta/dk$ is infinite at $k_\ast$.

3. $\beta_\ast$ is real and $k_\ast \geq 2\pi/L - \beta_\ast$. In this case, the zeroth, negative first, and probably more radiation channels are open. Assuming $\beta^\ast > 0$ as before, we have $\gamma_0 \to i\delta_0$ as $k \to k_\ast$, but since $\text{Im}(\beta^\ast_1 - k^2)$ is negative, $\gamma_1 \to -i\delta_{-1}$ where $\delta_{-1} = [k_\ast^2 - (\beta_\ast - 2\pi/L)^2]^{1/2} > 0$. Therefore, the limit solution $u_\ast$ contains an incoming plane wave for $m = 0$ and an outgoing plane wave for $m = -1$, and there is no outgoing wave in the zeroth diffraction channel and no incoming wave in the negative first diffraction channel. The existence of diffraction solutions with such a blazing property is well known [12]. Since $\beta$ also tends to $\beta_\ast$, the complex mode $\tau(r)$ also converges as $k \to k_\ast$. The limit of $\tau$ is the reciprocal diffraction solution of $u_\ast$. Its zeroth diffraction channel contains only incoming waves and the negative first diffraction channel contains only outgoing plane waves. Notice that $u$ and $\tau$ do not collapse to the same solution, and $d\beta/dk$ can be finite at $k_\ast$.

4. $\beta_\ast$ is complex with a nonzero $\text{Im}(\beta_\ast)$. In that case, $u_\ast$ is still a complex mode. Since a band of complex modes corresponds to $\beta$ being a differentiable function of $k$, we must have $\int_\Omega v_\ast \partial_y u_\ast \, dr = 0$, so that $d\beta/dk$ is infinite at $k_\ast$. It appears that this condition can only be satisfied when $\text{Re}(\beta_\ast) = 0$ or $\pi/L$ with two complex modes $u(r)$ and $v(r)$ converging to the same solution as $k \to k_\ast$.

For the three cases 1, 2 and 4, two complex modes, either $u$ and $\tau$ or $u$ and $v$, coalesce as $k \to k_\ast$. Therefore, these cases correspond to exceptional points (EPs) of the non-Hermitian eigenvalue problem for guided modes [16–20].

For a numerical example, we consider a periodic array of circular cylinders with radius $a = 0.3L$ and dielectric constant $\varepsilon_c = 15.42$, and show its band structure in Fig. 2. The periodic array has five bands of regular guided modes below the light line, and they are shown as the solid black curves in Fig. 2(a). The light line $k = \beta$ is shown as the red dashed line with a positive slope. Since the corresponding intervals for $\beta$ are small, the 4th and 5th bands are difficult to see in Fig. 2(a), but they are clearly shown in Fig. 2(d). All five bands start from the light line with a unit slope, i.e., $dk/d\beta = 1$, and end with a zero slope at $\beta = \pi/L$. The endpoints are marked by GM$_j$ for $1 \leq j \leq 5$ in Figs. 2(a) and (d). Except for the second band (with endpoint GM$_2$), the dispersion curves of the regular guide modes are increasing functions of $\beta$ for $\beta \in [0, \pi/L]$. In Fig. 2(c), we show the second dispersion curve near the light line. It is clear that the slope changes signs, and $k$ (as a function of $\beta$) has a local maximum at the point marked as EP$_1$.

The dispersion curves of the complex modes of this periodic array are also shown in Fig. 2. The solid blue curves in Fig. 2(a) depict six complex-mode bands ($k$ vs. $\text{Re}(\beta)$ only) with a varying $\text{Re}(\beta)$. Zoomed-in plots for the first and second bands near their right endpoints are shown in Figs. 2(c) and (d). Figure 2(b) shows several complex-mode bands with a fixed $\text{Re}(\beta) = \pi/L$. In Fig. 2, we show the real and imaginary parts of $\beta$ as functions of $k$ for the different complex-mode bands.

FIG. 2. Regular guided modes and complex modes on a periodic array of circular cylinders. (a): Regular guided modes with a real $\beta$ (solid black curves) and complex modes for varying $\text{Re}(\beta)$ (solid blue curves). (b) Complex modes for fixed $\text{Re}(\beta) = \pi/L$. (c) and (d): Zoomed-in plots near points A and B in (a), respectively.
than $k$ of the mode at $k > k^*$ be the freespace wavenumber and propagation constant $\beta^*$ coalescing to a regular guided mode. Let $v$ be the waveguides starting from the standing waves $SW_j$ for $1 \leq j \leq 6$ in Fig. 2(a). The panels with $EP_j$ ($j = 2, 3, 4$) include additional complex-mode bands with fixed $Re(\beta) = \pi/L$.

For all complex-mode bands in Fig. 2(a), as $k$ is decreased, $Re(\beta)$ increases. The right endpoint of the first complex-mode band is shown as $EP_1$ in Figs. 2(a) and (c), and it is exactly the local maximum on the second band of regular guided modes. Clearly, this endpoint corresponds to case 1, namely, two complex modes $u$ and $v$ coalescing to a regular guided mode. Let $k_*$ and $\beta_*$ be the freespace wavenumber and propagation constant of the mode at $EP_1$. For $k > k_*$, to represent a field in the waveguide that decays to zero as $y \to +\infty$, the two complex modes $u$ and $v$ with propagation constants $\beta = \beta' + i\beta''$ and $-\beta = -\beta' + i\beta''$, where $\beta'' > 0$) should be used in the eigenmode expansion. For $k$ slightly less than $k_*$, the periodic array has two guided modes $u_1$ and $u_2$ with propagation constants $\beta_1$ and $\beta_2$ satisfying $\beta_1 < \beta_* < \beta_2$. The periodic array also has two reciprocal modes $v_1$ and $v_2$ with propagation constants $-\beta_1$ and $-\beta_2$. Since the slopes at $\beta_1$ and $\beta_2$ have opposite signs, $u_1$ and $u_2$ carry power forward and backward, respectively. To represent a wave field that is outgoing as $y \to +\infty$, it is necessary to use $u_1$ and $u_2$ in the eigenmode expansion.

The right endpoints of second, third and fourth complex-mode bands shown in Fig. 2(a) have $Re(\beta_*) = \pi/L$ and $Im(\beta_*) \neq 0$, and they are marked as $EP_j$ for $2 \leq j \leq 4$ in Figs. 2(a), (b) and (d). In particular, the imaginary part of $\beta$, for these three endpoints are shown in Fig. 2(b). For $EP_4$, $Im(\beta_*)$ is small but still positive. Clearly, these endpoints correspond to case 4, i.e., two complex modes $u$ and $v$ merging to a degenerate complex mode with $Re(\beta_*) = \pi/L$ and $d\beta/dk$ tending infinity. For each $j \in \{2, 3, 4\}$, if $k_*$ is the freespace wavenumber of the complex mode at $EP_j$, then for $k < k_*$, two complex-mode bands with fixed $Re(\beta) = \pi/L$ emerge. In Fig. 2(b), there are three smooth curves containing $EP_2$, $EP_3$ and $EP_4$, respectively. On each curve, the value of $k$ reaches a local maximum (i.e., $k_*$) at $EP_j$. As $k$ is decreased from $k_*$, two complex modes with $Im(\beta) < Im(\beta_*)$ and $Im(\beta) > Im(\beta_*)$ (for $k$ close to $k_*$ only) emerge. Since $\beta$ is required to be a differentiable function of $k$ on a complex-mode band, each smooth curve containing one $EP_j$ in Fig. 2(b) corresponds to two complex-mode bands with $Re(\beta) = \pi/L$. One curve in Fig. 2(b) does not contain $EP_3$. Instead, it connects two regular guided modes $GM_1$ and $GM_2$. Notice that $GM_2$ is a local minimum of the second band of regular guided modes. All other $GM_j$ are local maxima of their corresponding bands.

As shown in Fig. 2(b), the six complex-mode bands starting from $EP_j$ for $2 \leq j \leq 4$, all end at points on the line $Im(\beta_*) = 0$. Since these bands have a fixed $Re(\beta) = \pi/L$, the lower endpoints of these bands all have the same propagation constant $\beta_*$ $= \pi/L$. It can be observed that the three bands with a decreasing $Im(\beta)$ (as $k$ is decreased from that of $EP_j$) exist only in very small intervals of $k$. For the other three bands, $Im(\beta)$ initially increases, but eventually decreases to zero. The lower endpoints of these six bands are either regular guided modes or special diffraction solutions with blazed properties. More specifically, the two bands emerging from $EP_2$ and one band emerging from $EP_4$ end at regular guided modes $GM_3$, $GM_4$ and $GM_5$, respectively. These endpoints correspond to case 1 discussed earlier. The two bands emerging from $EP_3$ end at diffraction solutions marked as $RM_5$ in Fig. 2(b). The tiny band to the left of $EP_4$ also ends at a diffraction solution with $\beta = \pi/L$. All these three diffraction solutions correspond to case 3. Let $u_*$ be any one of these solutions, then $u_*$ has only an incoming plane wave in the 0th diffraction order and only an outgoing plane wave in the $-1$st diffraction order. Since $\beta_0 = \beta_* = \pi/L = -\beta_{-1}$, the incoming and outgoing waves propagate exactly in opposite directions.

Finally, we consider the 5th and 6th complex-mode bands in Fig. 2(a). The right endpoints of these two bands are marked as $RM$ and also correspond to case 3.
The limiting solutions at these two endpoints are also blazing diffraction solutions that completely convert the power of the incoming waves in the 0th diffraction order to outgoing waves in the $-1$st diffraction order. But since $\beta_*$ (of the limiting diffraction solution) is less than $\pi/L$, we have $\beta_0 \neq -\beta_{-1}$, thus the incoming and outgoing plane waves have different incident angles.

In summary, we have found complex modes in an open lossless periodic waveguide. These modes are physical solutions that can be excited whenever the periodic waveguide has a discontinuity or a defect. The complex modes form bands on which the propagation constant $\beta$ is a complex-valued function of $k$. The bands may have a continuously varying Re($\beta$) or a fixed Re($\beta$) = $\pi/L$. At an end of a band, either the complex mode turns to a blazing diffraction solution, or a pair of complex modes merge to a regular guide mode, or a BIC, or a degenerate complex mode. Further studies are needed to develop a systematic approach for computing the complex modes, and to have a deeper understanding about the complex modes, including the number of bands and classification of the endpoints.

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