Computing diffraction anomalies as nonlinear eigenvalue problems

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When a plane electromagnetic wave impinges upon a diffraction grating or other periodic structures, reflected and transmitted waves propagate away from the structure in different radiation channels. A diffraction anomaly occurs when the outgoing waves in one or more radiation channels vanish. Zero reflection, zero transmission and perfect absorption are important examples of diffraction anomalies, and they are useful for manipulating electromagnetic waves and light. Since diffraction anomalies appear only at specific frequencies and/or wavevectors, and may require the tuning of structural or material parameters, they are relatively difficult to find by standard numerical methods. Iterative methods may be used, but good initial guesses are required. To determine all diffraction anomalies in a given frequency interval, it is necessary to repeatedly solve the diffraction problem for many frequencies. In this paper, an efficient numerical method is developed for computing diffraction anomalies. The method relies on nonlinear eigenvalue formulations for scattering anomalies and solves the nonlinear eigenvalue problems by a contour-integral method. Numerical examples involving periodic arrays of cylinders are presented to illustrate the new method.

I. INTRODUCTION

For diffraction gratings and other periodic structures, transmission and reflection spectra often have interesting and useful features, such as sharp peaks and dips, flat bands, and rapid variation from a peak to a dip [1–3]. For structures without material loss, especially when the structures have relevant symmetry, it is possible to have zero reflection (total transmission) or zero transmission (total reflection), for some special frequency and wavevector [4]. It is also widely observed that a peak and a dip may appear close to each other forming an asymmetric line shape, a phenomenon called Fano resonance [2–5]. For lossy periodic structures, a particular incident wave may induce no reflected and transmitted waves, giving rise to perfect absorption [6]. When there are more than one propagating diffraction orders, it is sometimes possible to force reflected (or transmitted) wave to a particular diffraction order, leading to the so-called blazing diffraction phenomenon [6]. These and other special diffraction conditions are often referred to as diffraction anomalies, and they have been extensively investigated both theoretically and experimentally [3].

To investigate their properties and realize their applications, efficient numerical methods are needed to calculate diffraction anomalies. The diffraction of a time-harmonic incident wave by a given periodic structure is a boundary value problem (BVP). Many numerical methods have been developed to solve this BVP [6–11]. Its general solution can be represented by a scattering matrix. As we shall show in Sec. II, every diffraction anomaly is equivalent to a condition on one or more entries of the scattering matrix. Therefore, the diffraction anomalies may be found by searching the frequency (or wavevector, or other parameters) iteratively. In each iteration, the BVP is solved to find some entries of the scattering matrix. Such an iterative scheme is widely used, but it may fail if good initial guesses are not available. In addition, if all diffraction anomalies (of certain type) in a given frequency range are required, it is necessary to densely scan the frequency interval. The problem becomes more complicated if the diffraction anomaly only exists when some structural parameters are properly tuned. Clearly, the existing method for computing diffraction anomalies is not very reliable and computationally expensive.

In this paper, we consider a few diffraction anomalies including zero reflection, zero transmission, perfect absorption and blazing diffraction, and reformulate all of them as a nonlinear eigenvalue problem (NEP)

\[
A(\omega)u = 0
\] (1)

where \(A\) is an operator that can be approximated by a square matrix, and \(\omega\) is the unknown frequency (the eigenvalue) that appears in \(A\) nonlinearly. For Eq. (1) to have a nonzero solution \(u\), the operator \(A(\omega)\) must be singular. This implies that \(\omega\) can be solved from conditions such as \(\det A(\omega) = 0\) or \(\sigma_1(A(\omega)) = 0\), where \(\sigma_1\) is the smallest singular value of \(A\). However, such a method also requires good initial guesses, and has similar disadvantages as the iterative method based on the scattering matrix. Our approach is to solve the NEP by the contour-integral method developed by Asakura et al. [12] and Beyn [13]. The method allows us to find all eigenvalues of Eq. (1) inside a closed contour in the complex plane of \(\omega\). Since no initial guesses are needed, the method is robust and reliable.

The rest of this paper is organized as follows. In Sec. II, we introduce the diffraction problem and scattering matrix, and identify the diffraction anomalies as special conditions on one or more entries of the scattering matrix. In Sec. III, the diffraction anomalies are reformulated as NEPs. Numerical examples for periodic arrays of circular cylinders are presented in Sec. IV. The paper is concluded with a few remarks in Sec. V.
II. DIFFRACTION ANOMALIES

In a two-dimensional (2D) structure that is translationally invariant in spatial variable \( x \), a polarized electromagnetic wave is also invariant in \( x \), and has only one nonzero component, namely the \( z \) component, in its electric or magnetic field. We consider an \( E \)-polarized time-harmonic electromagnetic wave in a 2D structure with a single periodic direction. The structure is periodic in \( y \), finite in \( z \), and surrounded by air. The dielectric function \( \varepsilon \) of the structure satisfies
\[
\varepsilon(y + L, z) = \varepsilon(y, z), \quad \forall (y, z) \in \mathbb{R}
\]
where \( L \) is the period in the \( y \) direction and \( 2d \) is the thickness of the structure. The structure is periodic in \( x \), and the associated plane wave is the wavevector \( \beta = \omega/c \) where \( \omega = c \varepsilon_0 \) is the angular frequency, \( c \) is the speed of light in vacuum, and the time dependence is \( e^{-i\omega t} \).

A diffraction problem can have one or more plane incident waves illuminating on the periodic structure. We assume the incident waves are associated with a fixed frequency \( \omega \) and a fundamental wavenumber \( \beta \in (-\pi/L, \pi/L) \) for the \( y \) direction. Due to the periodicity, for any integer \( m \), \( \beta_m = \beta + 2\pi m/L \) is a compatible wavenumber, and the associated plane wave is the \( m \)-th diffraction order. For each integer \( m \), \( \gamma_m = \sqrt{k_0^2 - \beta_m^2} \) is either real (non-negative) or pure imaginary. We assume there is a set of integers \( M \) containing 0, such that if \( m \in M \) then \( \gamma_m > 0 \), if \( m \notin M \) then \( \gamma_m = i\mu_m \) for \( \mu_m > 0 \). For \( m \in M \) and \( m \notin M \), the plane waves with wavevectors \( (\beta_m, \pm\gamma_m) \) are propagating and evanescent diffraction orders, respectively. The diffraction problem can be studied with incident waves containing all propagating diffraction orders and given above and below the periodic layer (i.e. for \( z > d \) and \( z < -d \), respectively). For \( |z| \geq d \), we can write down the solution of a diffraction problem as
\[
u(y, z) = u_{\text{inc}}^+(y, z) + u_{\text{sca}}^+(y, z), \quad \pm z \geq d,
\]
where the superscripts “+” and “−” signify waves above and below the periodic layer, respectively, and the subscripts indicate incident and scattered waves, respectively. Moreover, the incident and scattered waves can be expanded in plane waves as
\[
u_{\text{inc}}^\pm(y, z) = \sum_{m \in \mathbb{M}} a_m^\pm e^{i(\beta_m y + \gamma_m z)},
\]
\[
u_{\text{sca}}^\pm(y, z) = \sum_{m \in \mathbb{Z}} b_m^\pm e^{i(\beta_m y + \gamma_m z)},
\]
where \( Z \) is the set of all integers, \( a_m^\pm \) for \( m \in \mathbb{M} \), are given coefficients of the incident plane waves, and \( b_m^\pm \) for all \( m \), are the coefficients of the outgoing propagating or evanescent plane waves.

The scattering matrix \( S \) maps the coefficients of the incident waves to the coefficients of the outgoing propagating waves, namely
\[
\begin{bmatrix} b^+ \\ b^- \end{bmatrix} = S \begin{bmatrix} a^+ \\ a^- \end{bmatrix},
\]
where \( a^+ \) is a column vector of \( a_m^+ \) for all \( m \in \mathbb{M} \), \( b^+ \) is a column vector of \( b_m^+ \) for all \( m \in \mathbb{M} \), etc. Let \( M \) be the number of integers in \( \mathbb{M} \), then \( S \) is a \( (2M) \times (2M) \) square matrix. It is clear that \( S \) depends on the frequency \( \omega \) and the wavenumber \( \beta \). If the periodic structure has no material loss, \( \varepsilon(y, z) \) is a real positive function, then energy is conserved and \( S \) is a unitary matrix.

The simplest and most important case is \( M = \{0 \} \), namely, the zeroth diffraction order is the only propagating order. In that case, \( S \) is a \( 2 \times 2 \) matrix satisfying
\[
\begin{bmatrix} b_0^+ \\ b_0^- \end{bmatrix} = S \begin{bmatrix} a_0^+ \\ a_0^- \end{bmatrix}.
\]
Let \( s_{jk} \) be the \( (j, k) \) entry of above \( S \). If for a fixed \( \beta \), \( s_{11}(\omega) = 0 \) for a real frequency \( \omega \), then for an incident wave given above the periodic layer, there is no reflected wave. This is the simplest case of zero reflection and it is considered as a diffraction anomaly. If the structure is lossless, the unitarity of \( S \) implies \( |s_{21}(\omega)| = 1 \), thus, zero reflection implies total transmission. Similarly, if \( s_{21}(\omega) = 0 \), then \( \omega \) is the frequency for zero transmission for an incidence wave given above the periodic layer. If the periodic structure is lossless, zero transmission implies total reflection. We also regard zero transmission as a diffraction anomaly. Popov et al. [4] first realized that structural symmetry is important to the appearance of zero reflection and zero transmission. In some cases, the frequency for these anomalies can be approximated [4, 6, 17, 18]. However, even for periodic structures with the right symmetry, the existence of zero reflection/transmission has only been rigorously established for special circumstances [13, 20].

For lossless structures, the power of incident waves is completely converted to outgoing waves. For \( M = 1 \), that means \( |a_0^+|^2 + |a_0^-|^2 = |b_0^+|^2 + |b_0^-|^2 \). If the structure has material loss, i.e., \( \text{Im}(\varepsilon) \) is positive somewhere, there could be a real frequency \( \omega \) such that \( b_0^+ = b_0^- = 0 \) for some \( (a_0^+, a_0^-) \neq (0, 0) \). This is a case of perfect absorption [4, 21, 22] or coherent perfect absorption [23], and it is a useful diffraction anomaly for solar cell technology. Notice that perfect absorption corresponds to \( S(\omega) \) being a singular matrix, and thus \( \det S(\omega) = 0 \).

If there are two propagating diffraction orders, i.e., \( M = 2 \), then \( S \) is a \( 4 \times 4 \) matrix. For \( \beta \in (0, \pi/L) \), we have \( M = \{0, -1\} \), namely, the propagating orders correspond to wavenumbers \( \beta_0 = \beta \) and \( \beta_{-1} = \beta - 2\pi/L \). We are interested in a diffraction anomaly where incident waves are given in the zeroth diffraction order and outgoing waves appear in the \(-1\)st diffraction order only. To
write down a condition for this blazing diffraction phenomenon [7], we assume vectors $a^\pm$ and $b^\pm$ are
\[ a^\pm = \begin{bmatrix} a^\pm_{-1} \\ a^\pm_0 \end{bmatrix}, \quad b^\pm = \begin{bmatrix} b^\pm_{-1} \\ b^\pm_0 \end{bmatrix}, \] (10)
and the entries of $S$ are $s_{jk}$ for $1 \leq j, k \leq 4$. The scattering matrix satisfies
\[ \begin{bmatrix} b^\pm_{-1} \\ 0 \\ b^\pm_{-1} \\ 0 \end{bmatrix} = S \begin{bmatrix} 0 \\ a^+_0 \\ 0 \\ a^-_0 \end{bmatrix}. \] (11)
The 2nd and 4th rows of above give
\[ \begin{bmatrix} s_{22} & s_{24} \\ s_{42} & s_{44} \end{bmatrix} \begin{bmatrix} a^+_0 \\ a^-_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \] (12)
Therefore,
\[ \det \begin{bmatrix} s_{22} & s_{24} \\ s_{42} & s_{44} \end{bmatrix} = 0. \] (13)

In summary, we have considered diffraction anomalies including zero reflection, zero transmission, perfect absorption and blazing diffraction. In terms of the scattering matrix, each anomaly corresponds to a zero condition on an entry or a sub-matrix of the scattering matrix. The diffraction anomalies may occur at a specific frequency $\omega$ for a fixed structure and a fixed wavenumber $\beta$. In that case, all we have to do is to calculate $\omega$ by solving a scalar equation. If the incident angle is fixed, then $\beta$ is related to $\omega$, and the frequency is still the only unknown. Diffraction anomalies can also be studied for a fixed frequency, then the wavenumber $\beta$ or incident angle is the unknown. However, for a fixed structure, some diffraction anomalies may not occur for any frequency or wavenumber. In that case, it is necessary to add tunable parameters to the structure, and solve the parameters together with the frequency and/or wavenumber.

In principle, we can find diffraction anomalies by solving the equations obtained from the scattering matrix. Such a method works well if there are good initial guesses, but since good initial guesses are not easy to obtain, the method is not robust. Moreover, the method becomes computationally expensive if all diffraction anomalies in a given frequency or wavenumber interval are required. To obtain good initial guesses, it is necessary to densely scan the frequency or wavenumber interval. This implies that the diffraction problem must be solved repeatedly for many different values of the frequency or wavenumber, and this is computationally expensive.

III. NONLINEAR EIGENVALUE FORMULATIONS

To overcome the difficulty of finding good initial guesses for all diffraction anomalies in a given frequency/wavenumber interval, we develop a robust numerical method based on nonlinear eigenvalue formulations and a contour-integral method for solving nonlinear eigenvalue problems [13–16]. Although the diffraction of a time-harmonic wave is a BVP, the diffraction anomalies are special conditions of this BVP, and they can be reformulated as eigenvalue problems where the eigenvalue is the frequency or wavenumber. However, the eigenvalue problem is nonlinear with a nonlinearity in the eigenvalue. Fortunately, this type of nonlinear eigenvalue problems (NEPs) can be accurately and robustly solved by the contour-integral method [13–14].

To describe the NEP formulations for various diffraction anomalies, we first consider the standard eigenvalue problem for resonant modes [24, 25], and reformulate this linear eigenvalue problem as a NEP. In a 2D periodic structure given by a dielectric function $\epsilon(y, z)$ satisfying conditions (2) and (3), any $E$-polarized eigenmode is a Bloch mode
\[ u(y, z) = \phi(y, z)e^{i\beta z}, \] (14)
where $\phi$ is periodic in $y$ with period $L$ and $\beta$ is the Bloch wavenumber. The eigenvalue problem is for $u$ satisfying Eq. (4) and proper boundary conditions as $z \to \pm \infty$. The eigenvalue is either $\omega$ (or $k_0 = \omega/c$, or $k_0^2$) for given real $\beta \in (-\pi/L, \pi/L)$, or $\beta$ for given $\omega > 0$. We focus on the case where $\omega$ is the eigenvalue. If the boundary condition is $u \to 0$ as $z \to \pm \infty$, then the eigenmode is a guided mode. We are concerned with resonant modes (also called resonant states or quasi-normal modes) for which $u$ satisfies an outgoing radiation condition as $z \to \pm \infty$ [24, 25]. This condition implies that power is radiated out to infinity as $z \to \pm \infty$, and $\omega$ must have a negative imaginary part, so that the mode amplitude decays with time.

For $|z| > d$, the nonzero electric field component of a resonant mode can be expanded in plane waves, exactly like $u^\pm_{scu}$ in Eq. (7), namely,
\[ u(y, z) = \sum_{m \in \mathbb{Z}} c_m^\pm e^{i(\beta_m y \pm \gamma_m z)}, \quad \pm z \geq d, \] (15)
where $c_m^\pm$ are the expansion coefficients, $\beta_m$ and $\gamma_m$ are given in Sec. II. However, $k_0$ is now complex with a negative imaginary part, $k_0^2 - \beta_m^2$ is in the lower half of the complex plane, the complex square root in
\[ \gamma_m = \sqrt{k_0^2 - \beta_m^2} \] (16)
should be defined using a branch cut along the negative imaginary axis (instead of the negative real axis), so that when $k_0^2 - \beta_m^2$ is in the third or fourth quadrant, $\gamma_m$ is in the second or fourth quadrant, respectively. This choice of complex square root ensures that each term in the right hand side of Eq. (15) is either an evanescent plane wave that decays exponentially as $z \to \pm \infty$, or an outgoing plane wave that radiates out power (and grows exponentially) as $z \to \pm \infty$. As in Sec. II, we have a set
$M$ for those integers $m$ such that $k_0^2 - \beta_m^2$ is in the fourth quadrant. We assume $M$ is not empty and contains 0. In that case, the resonant mode has the following far field asymptotic expansion

$$u(y, z) \sim \sum_{m \in \mathbb{M}} c_m^e e^{i(\beta_m y + \gamma_m z)}, \quad z \to \pm \infty.$$  

(17)

The linear eigenvalue problem of a resonant mode is for $u$ satisfying Eq. (1) in $\Omega_{\text{in}}$, the far field condition (17), and the following quasi-periodic conditions

$$\begin{bmatrix} u \\ \partial_y u \end{bmatrix} \big|_{y = L} = e^{i\beta L} \begin{bmatrix} u \\ \partial_y u \end{bmatrix} \big|_{y = 0},$$

(18)

where $\Omega_{\text{in}}$ is given by $0 < y < L$ and $-\infty < z < \infty$. Since the coefficients $c_m^e$ for $m \in \mathbb{M}$ are unknown, the far field condition (17) is difficult to use. The standard approach is to use the perfectly matched layer (PML) technique [26–28], namely, move $z$ to a path in the complex plane so that $u(y, z) \to 0$ as $z \to \infty$ along the path.

If we define a linear operator $A_0$ such that

$$A_0 e^{i\beta_m y} = i\gamma_m e^{i\beta_m y}, \quad m \in \mathbb{Z},$$

(19)

then Eq. (15) gives rise to

$$\frac{\partial u}{\partial z} = A_0 u, \quad z = d,$$

(20)

$$\frac{\partial u}{\partial z} = -A_0 u, \quad z = -d.$$ 

(21)

The operator $A_0$ maps $u$ (Dirichlet data) to the derivative of $u$ (Neumann data), and is a so-called Dirichlet-to-Neumann (DtN) operator. Since $A_0$ depends on $\omega$ and $\beta$, we obtain a NEP for $u$ satisfying Eq. (1) in $\Omega_{\text{in}}$, and boundary conditions (13), (24) and (25), where $\Omega_d$ is the rectangular domain given by $0 < y < L$ and $-d < z < d$.

The above NEP formulation on $\Omega_d$ can be used for numerical implementation, but we prefer a NEP formulated on two line segments at $z = \pm d$ (for $0 < y < L$). To achieve this, we define a linear operator $F$ that maps $u$ at $z = \pm d$ (as functions of $y$ for $0 < y < L$) to $\partial_z u$ at $z = \pm d$, where $u$ satisfies Eq. (10) and boundary condition (18). The operator $F$ depends on both $\beta$ and $\omega$, and satisfies

$$F u = \begin{bmatrix} \partial_z u(y, d) \\ \partial_z u(y, -d) \end{bmatrix}, \quad u = \begin{bmatrix} u(y, d) \\ u(y, -d) \end{bmatrix}.$$ 

(22)

Let $F$ be given in $2 \times 2$ blocks,

$$F = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix},$$

(23)

then Eqs. (20), (22) lead to Eq. (1), where $A = A(\omega)$ is the $2 \times 2$ matrix operator

$$A = \begin{bmatrix} F_{11} - A_0 & F_{12} \\ F_{21} & F_{22} + A_0 \end{bmatrix}.$$ 

(24)

Equation (1) with the above $A$ is our preferred NEP formulation for resonant modes. For given $\omega$ and $\beta$, the two operators $A_0$ and $F$ can be approximated by matrices. If $y \in (0, L)$ is discretized by $N$ points, then $u$ is approximated by a column vector of length $2N$, $A_0$ and $F$ are approximated by $N \times N$ and $(2N) \times (2N)$ matrices, respectively. In Appendix, we give additional details on computing the matrix approximations of $A_0$ and $F$.

Next, we present NEP formulations for diffraction anomalies discussed in Sec. II. First, we consider a zero reflection where the incident wave is given above the periodic layer (i.e., for $z > d$) in the zeroth diffraction order and there is no reflected wave in the same diffraction order. Therefore, the total field for $|z| > d$ can be expanded as follows:

$$u = a_0^+ e^{i(\beta_0 y - \gamma_0 z)} + \sum_{m \neq 0} b_m^+ e^{i(\beta_m y + \gamma_m z)}, \quad z > d,$$

(25)

$$u = \sum_{m \neq 0} b_m^- e^{i(\beta_m y - \gamma_m z)}, \quad z < -d.$$ 

(26)

Clearly, $u$ satisfies Eq. (21), the same boundary condition as the resonant modes, at $z = -d$. To obtain a boundary condition at $z = d$, we define a new linear operator $A_1$ by

$$A_1 e^{i\beta_m y} = \begin{cases} -i\gamma_0 e^{i\beta_0 y}, & m = 0, \\ i\gamma_m e^{i\beta_m y}, & m \neq 0, \end{cases}$$

(27)

then $u$ satisfies

$$\frac{\partial u}{\partial z} = A_1 u, \quad z = d.$$ 

(28)

Therefore, the NEP for zero reflection is Eq. (1) with a new matrix operator $A$ given by

$$A = \begin{bmatrix} F_{11} - A_1 & F_{12} \\ F_{21} & F_{22} + A_0 \end{bmatrix}.$$ 

(29)

The case of zero transmission is somewhat more complicated. If an incident wave is given above the periodic layer in the zeroth diffraction order, and there is no transmitted wave in the zeroth diffraction order below the layer, then the total field is

$$u = a_0^+ e^{i(\beta_0 y - \gamma_0 z)} + \sum_{m \neq 0} b_m^+ e^{i(\beta_m y + \gamma_m z)}, \quad z > d,$$

(30)

$$u = \sum_{m \neq 0} b_m^- e^{i(\beta_m y - \gamma_m z)}, \quad z < -d.$$ 

(31)

Because of the incident wave, the boundary condition at $z = d$ is inhomogeneous. We have

$$\frac{\partial u}{\partial z} = A_0 u - 2ia_0^+ \gamma_0 e^{i(\beta_0 y - \gamma_0 d)}, \quad z = d.$$ 

(32)
Although \( b_0 = 0 \), \( u \) still satisfies Eq. (21) at \( z = -d \). The condition \( b_0 = 0 \) implies that

\[
\int_0^L u(y, -d)e^{-i\beta_0 y} dy = 0. \tag{33}
\]

Combining the above with the operator \( F \), we obtain a NEP given as Eq. (1) with a new matrix operator

\[
A = \begin{bmatrix}
F_{11} - \Lambda_0 & F_{12} \\
F_{21} & F_{22} + \Lambda_0
\end{bmatrix}, \tag{34}
\]

and a new vector

\[
u = \begin{bmatrix}
u(y, d) \\
u(y, -d)
\end{bmatrix}, \tag{35}
\]

where \( f(y) = 2ia_0^+\gamma_0e^{i(\beta_0 y - \gamma_0d)} \), and \( g \) is the linear functional that maps \( u(y, -d) \) to the left hand side of Eq. (33). When \( y \in (0, L) \) is discretized by \( N \) points, \( f(y) \) becomes by a column vector of length \( N \), \( g \) is approximated by a row vector of length \( N \), and \( A \) becomes a \((2N + 1) \times (2N + 1)\) matrix.

When the structure is absorptive, we can consider perfect absorption for which some incident waves do not produce any outgoing propagating waves. If there is only one propagating diffraction order for each side of the periodic layer, the total field can be written as

\[
u = a_0^+e^{i(\beta_0 y - \gamma_0z)} + \sum_{m \neq 0} b_m^+e^{i(\beta_m y + \gamma_m z)}, \quad z > d, \tag{36}
\]

\[
u = a_0^-e^{i(\beta_0 y + \gamma_0z)} + \sum_{m \neq 0} b_m^-e^{i(\beta_m y - \gamma_m z)}, \quad z < -d. \tag{37}
\]

Therefore, the boundary condition at \( z = d \) is Eq. (28), same as the zero reflection case considered above. The boundary condition at \( z = -d \) is

\[
\frac{\partial \nu}{\partial z} = -\Lambda_1 \nu, \quad z = -d. \tag{38}
\]

Therefore, the NEP for perfect absorption is Eq. (1) with \( \nu \) given in (22), and \( A \) given by

\[
A = \begin{bmatrix}
F_{11} - \Lambda_1 & F_{12} \\
F_{21} & F_{22} + \Lambda_1
\end{bmatrix}. \tag{39}
\]

For a lossless periodic structure, and if there are two propagating diffraction orders (the zeroth and negative-first orders if \( 0 < \beta \leq \pi/L \)), we can consider a blazing diffraction phenomenon that converts all power of the incident waves (in zeroth diffraction order) to outgoing waves in the negative first order. The total field for \( |z| > d \) has the same expansions (36) and (37). Therefore, the NEP formulation is also Eq. (1) with \( A \) given in Eq. (39) and \( \nu \) given in (22).

### IV. NUMERICAL EXAMPLES

To illustrate our method, we consider a periodic array of dielectric cylinders surrounded by air. The radius and the dielectric constant of the cylinders are \( a \) and \( \epsilon_1 \), respectively. The cylinders are parallel to the \( x \) axis. Their centers are located on the \( y \) axis. The period \( L \) of the array is the distance between the centers of two nearby cylinders. The array is considered as a periodic layer with a thickness \( 2d = L \). For all numerical examples, we discretize the interval \((0, L)\) by \( N = 11 \) points. Therefore, the operators \( \Lambda_0 \) and \( \Lambda_1 \) are approximated by \((11 \times 11)\) matrices, and the operator \( F \) is approximated by a \( 22 \times 22 \) matrix, and the matrix \( A \) is either \( 22 \times 22 \) or \( 23 \times 23 \). When the contour-integral method is used to solve the NEP, we use 100 points to discretize the contour and approximate integrals along the contour by the trapezoid method.

First, we consider the periodic array with \( a = 0.3L \) and \( \epsilon_1 = 11.6 \). In Fig. 1, we show the transmission spectra for a plane incident wave with wavenumber \( \beta = 0 \) (normal incidence) and \( \beta = 0.2/L \), respectively. The incident wave is given above the array, thus \( a_0^+ \neq 0 \), \( a_0^- = 0 \), and the transmission coefficient is \( T_0 = s_{21} = b_0^-/a_0^+ \). From Fig. 1 it appears that total transmission (zero reflection) and zero transmission occur at some special frequencies. To find the frequencies for zero reflection/transmission and the resonant modes, we use the contour-integral method with a circular contour in the complex plane of \( \omega \) centered on the real axis. In Table 1, we show seven resonant modes for \( \beta = 0 \) and \( \beta = 0.2/L \), respectively. The results are obtained using a contour with center at \( 0.7(2\pi c/L) \) and radius \( 0.2(2\pi c/L) \). Notice that for \( \beta = 0 \),

![FIG. 1. Transmission spectra of a periodic array of circular cylinders](image-url)
TABLE I. Frequencies of resonant modes in a periodic array of circular cylinders with \(a = 0.3L\) and \(\epsilon_1 = 11.6\), for wavenumber \(\beta = 0\) and 0.2/L.

| \(\omega L/(2\pi c)\) for \(\beta = 0\) | \(\omega L/(2\pi c)\) for \(\beta = 0.2/L\) |
|---------------------------------|---------------------------------|
| 0.557333 - 0.002047i           | 0.557898 - 0.002502i           |
| 0.589733                        | 0.589439 - 0.000147i           |
| 0.593629 - 0.058809i            | 0.593758 - 0.058677i           |
| 0.770917 - 0.002940i            | 0.771034 - 0.002876i           |
| 0.784154                        | 0.784059 - 0.000061i           |
| 0.858999                        | 0.857857 - 0.000543i           |
| 0.857873 - 0.054473i            | 0.857930 - 0.054206            |

there are three special resonant modes with a real frequency. They are examples of bound states in the continuum (BICs)\(^{29,50}\). A BIC has the same expansion, Eq. (15), as the resonant modes, but \(c_{\beta m}^2 = 0\) for any \(m\) such that \(\gamma_m\) is real. For the three BICs in Table II since \(M = \{0\}\), only \(c_{\beta 0}^2 = 0\). Although a BIC does not radiate out power as \(z \rightarrow \pm \infty\), it satisfies the same boundary conditions and the same NEP formulation as the resonant modes. The three BICs in Table II are standing waves with \(\beta = 0\), and they turn to resonant modes with a high \(Q\) factor as \(\beta\) moves away from zero.

In Table III we list zero-reflection frequencies for both \(\beta = 0\) and \(\beta = 0.2/L\). The NEP for zero transmission, i.e. Eq. 1 for \(A\) given in 43, is also satisfied by the BICs, but unlike that given in Eq. 39, for a BIC, the last entry of \(u\) is zero. For \(\beta = 0\), the numerical results include two zero-transmission frequencies listed in Table III and four BICs [three listed in Table II and a new one with frequency \(\omega = 0.411228(2\pi c/L)\)]. Of course, the computed vector \(u\) is scaled differently, its last entry is not simply 1 or 0. However, the BICs can be easily identified by considering the ratio between the last entry and the entry with the maximum magnitude. In our case, the ratio for the four BICs ranges from \(O(10^{-9})\) to \(O(10^{-7})\). The contour-integral method generally gives complex solutions for \(\omega\). For the two zero-transmission frequencies of \(\beta = 0\) in Table III, the imaginary part of the normal-frequency \(\omega L/(2\pi c)\) is \(O(10^{-11})\). For \(\beta = 0.2/L\), the numerical solutions are less accurate, but \(\text{Im}(\omega L/(2\pi c))\) is still bounded by \(4.4 \times 10^{-5}\) for all cases listed in the right column of Table III.

Next, we consider perfect absorption of normal incident waves (\(\beta = 0\)) in a periodic array of circular cylinders with material loss, where \(\epsilon_1\) (the dielectric constant of the cylinders) is complex. However, for a fixed \(\epsilon_1\) and a fixed radius \(a\), perfect absorption does not usually occur, and the NEP problem for \(A\) given in 43, has only complex-\(\omega\) solutions. To find perfect absorption for the periodic array, we have to tune a structural or material parameter. For example, if \(a = 0.3L\) is fixed and the refractive index of the cylinders is \(n_1 = \sqrt{\epsilon_1} = \sqrt{1.6} + i\sigma\), where \(\sigma\) is a parameter, then perfect absorption occurs at \(\sigma = 0.0142765\) with a real frequency \(\omega = 0.770981(2\pi c/L)\). This result is obtained iteratively with an iteration in \(\sigma\). In each iteration (i.e. for a given \(\sigma\)), we solve the NEP using a circular contour (in the complex \(\omega\) plane) with center \(0.8(2\pi c/L)\) and radius \(0.1(2\pi c/L)\) and find a solution \(\omega\) which is complex in general. The iterative process can be regarded as a root-finding method for solving \(\text{Im}(\omega) = 0\). We can also find perfect absorption by tuning the radius \(a\) for a fixed complex \(\epsilon_1\). In Table IV we list a few cases where the imaginary part of \(n_1\) is specified. The results are obtained using a circular contour with center \(0.7(2\pi c/L)\) and radius 0.2(2\pi c/L).
Finally, we consider blazing diffraction for a periodic array of cylinders with radius $a = 0.3L$ and dielectric constant $\epsilon_1 = 15.42$, and concentrate on the case of two propagating diffraction orders with wavenumbers $\beta = \beta_0 = \pi/L$ and $\beta_{-1} = -\pi/L$. Using a circular contour with center $0.65(2\pi c/L)$ and radius $0.11(2\pi c/L)$, we find the following five frequencies

$$0.549336, 0.670542, 0.678285, 0.686822, 0.745395.$$  

Since the periodic array has a mirror symmetry in $z$, the blazing diffraction solutions are either even or odd in $z$. Among the five solutions above, the first three are even in $z$ and the last two are odd in $z$.

We have repeated some calculation using different values of $N$ [for discretizing the interval $(0, L)$] and different number of points for discretizing the contour. Typically, $N = 9$ is sufficient to give four significant digits. When $N$ is increased to 11, the accuracy is improved by at least a factor of two. For discretizing the contour, 100 points is more than enough. Typical numerical results obtained with 100 and 200 points for the contour have more than eight identical digits.

| $\sigma = \text{Im}(n_1)$ | $a/L$ | $\omega L/(2\pi c)$ |
|-----------------------------|-------|---------------------|
| 0.012                       | 0.322575 | 0.715869 |
| 0.013                       | 0.312982 | 0.738371 |
| 0.014                       | 0.302888 | 0.763499 |
| 0.015                       | 0.292248 | 0.791757 |

V. CONCLUSION

Diffraction anomalies such as zero reflection, zero transmission, perfect absorption and blazing diffraction are interesting wave phenomena with important applications. Existing methods for computing the diffraction anomalies either scan the frequency (or wavenumber, or other parameters) densely or determine the frequency iteratively, and thus, they are computationally expensive and not very reliable. Our method based on NEP formulations and a contour-integral method is capable of finding all diffraction anomalies in a given frequency interval. Since the NEPs involve small matrices and no initial guesses for the frequency are needed, our method is efficient and robust. Although the method is only formulated for $E$-polarized waves in 2D structures with a single periodic direction, it can be easily generalized to full-vector waves in 3D structures with two periodic directions. It is also straightforward to extend the method to other diffraction anomalies. The method provides a useful tool for analyzing diffraction anomalies and explore their applications.

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Appendix: Matrix approximation of $A_0$ and $F$

Here, we briefly describe how operators $A_0$ and $F$ can be approximated by matrices, if the structure is a periodic array of circular cylinders surrounded by air. Let $L$ be the period of the array, $a$ and $n_1$ be the radius and refractive index of the cylinders, respectively. For $d = L/2$, $\Omega_d$ is a square given by $0 < y < L$ and $-d < z < d$. We assume a cylinder is contained in $\Omega_d$ and centered at $(y, z) = (L/2, 0)$.

Let $N = 2p + 1$ be a positive odd integer and $y_j = (j - 0.5)/L$ for $1 \leq j \leq N$. For $z \geq d$, the field expansion may be approximated by

$$u(y, z) \approx \sum_{m=-p}^{p} c_m^+ e^{i(\beta m y + \gamma_m z)}, \quad z \geq d. \quad (A.1)$$

Evaluating the above at $(y, z) = (y_j, d)$, we obtain an $N \times N$ matrix $C_1$, such that

$$u^+ \approx C_1 c^+,$$

where $u^+$ is a column vector of $u(y_j, d)$ for $1 \leq j \leq N$, and $c^+$ is a column vector of $c_m^+$ for $-p \leq m \leq p$. We can also take a derivative with respect to $z$ for the approximate expansion above and evaluate the result at $(y_j, d)$ for $1 \leq j \leq N$. This gives rise to a matrix $C_2$ such that

$$\partial_z u^+ \approx C_2 c^+,$$

where $\partial_z u^+$ is a vector for $\partial_z u(y_j, d)$. The operator $A_0$ is then approximated by the $N \times N$ matrix $C_2 C_1^{-1}$.

Inside $\Omega_d$, the general solution Eq. (1) is

$$u(y, z) = \sum_{m=-\infty}^{+\infty} d_m \phi_m(r) e^{im\theta}, \quad (A.2)$$

where $(r, \theta)$ are the polar coordinates satisfying

$$y = L/2 + r \cos \theta, \quad z = r \sin \theta,$$

and $\phi_m$ is a particular solution with a cylindrical wave incident upon the cylinder. More specifically, $\phi_m(r) = A_m J_m(k_0 n_1 r)$ for $r < a$ and $\phi_m(r) = B_m H_m^{(1)}(k_0 r) + H_m^{(2)}(k_0 r)$ for $r > a$, where $J_m$, $H_m^{(1)}$, $H_m^{(2)}$ are $m$-th order Bessel and Hankel functions. The coefficients $A_m$ and $B_m$ can be solved from the condition that $\phi_m$ and $d\phi_m/dr$ are continuous at $r = a$. Now, we approximate the expansion by $4N$ terms:

$$u(y, z) \approx \sum_{m=-2N}^{2N-1} d_m \phi_m(r) e^{im\theta}. \quad (A.3)$$
From the above, we can take partial derivatives and find the approximate expansions for $\partial_y u$ and $\partial_z u$. Let $z_k = -L/2 + (k - 0.5)/L$ for $k = 1, 2, ..., N$. Evaluating $u$ by Eq. (A.3) at $(y_j, d)$, $(y_j, -d)$ for $1 \leq j \leq N$ and $(0, z_k)$ and $(L, z_k)$ for $1 \leq k \leq N$, we obtain a $(4N) \times (4N)$ matrix $D_1$ mapping a column vector $d$ (for $d_m = -2N \leq m < 2N - 1$) to a column vector of length $4N$ for $u$ at the $4N$ sampling points on the boundary of $\Omega_d$. Similarly, we can evaluate $\partial_y u$ at $(y_j, \pm d)$ for $1 \leq j \leq N$ and evaluate $\partial_y u$ at $(0, z_k)$ and $(L, z_k)$ for $1 \leq k \leq N$, and obtain a $(4N) \times (4N)$ matrix $D_2$ that maps vector $d$ to a vector of length $4N$ for the normal derivative of $u$ at the $4N$ points on the boundary of $\Omega_d$. Therefore, $D_2 D_1^{-1}$ is a $(4N) \times (4N)$ matrix mapping $u$ to the normal derivative of $u$ at the $4N$ points on the boundary of $\Omega_d$. Finally, we can use the quasi-periodic condition to eliminate $u$ and $\partial_y u$ at $y = 0$ and $y = L$. The final result is a $(2N) \times (2N)$ matrix $F$ satisfying

$$\begin{bmatrix} \partial_z u^+ \\ \partial_z u^- \end{bmatrix} = F \begin{bmatrix} u^+ \\ u^- \end{bmatrix},$$

(A.4)

where $u^-$ and $\partial_z u^-$ are column vectors of $u(y_j, -d)$ and $\partial_z u(y_j, -d)$ for $1 \leq j \leq N$, respectively.

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