Approximating transmission and reflection spectra near isolated nondegenerate resonances

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A linear scattering problem for which incoming and outgoing waves are restricted to a finite number of radiation channels, the complete solution of any linear scattering problem is given by a finite scattering matrix that maps the amplitudes of the incoming waves to those of the outgoing waves. Typically, the incoming and outgoing waves are time-harmonic waves and the scattering matrix depends on the frequency. Entries of the scattering matrix, as functions of the frequency, can be used to find the transmission and reflection spectra. As first observed by Wood [1], transmission and reflection spectra often exhibit rapid variations with sharp peaks and/or dips. In numerous applications, a peak and a dip appear in a narrow frequency range forming an asymmetric line shape—a phenomenon called Fano resonance [2–5]. For structures without absorption loss and with a proper symmetry, the peaks and dips can actually reach 100% and 0, respectively [4, 6–9]. It is widely accepted that Fano resonance is the consequence of interference between a direct (non-resonant) passway and a resonance-assisted indirect pathway [5]. In photonics, Fano resonance has found many applications including filtering, sensing and switching [6–13].

To find the scattering matrix rigorously, it is necessary to solve the governing partial differential equation (PDE), such as the Maxwell’s equations for electromagnetic waves. Accurate numerical solutions for a large frequency range are expensive to obtain and do not provide much physical insight. To improve the understanding on resonant scattering phenomena, it is desirable to derive analytic models for scattering matrices and transmission/reflection spectra. A good analytic model should reveal the most important physical phenomena and predict the peaks and dips in transmission/reflection spectra. The temporal coupled-mode theory (TCMT) is a simple system (for the amplitudes of the resonant modes and incoming and outgoing waves) constructed by considering energy conservation, reciprocity and time-reversal symmetry [6, 14–16]. Although it is not derived from the governing PDE, TCMT produces a simple model for the scattering matrix and predicts the peaks and dips accurately. To use the TCMT for any specific application, it is necessary to find the resonant mode and estimate the scattering matrix $C$ for the direct passway. While the resonant mode can be solved from the governing PDE, the scattering matrix $C$ cannot be solved rigorously. A different modeling approach, first suggested by Popov et al. [4], is to approximate the entries of the scattering matrix by simple rational functions based on their poles and zeros in the complex plane [4, 14–21]. It is well-known that the complex frequency of a resonant mode is a pole of the scattering matrix. Each entry of the scattering matrix has its own zeros and they are complex in general. In case a dip in a transmission or reflection spectrum is actually 0, the corresponding entry in the scattering matrix has a real zero. Both poles and zeros can be found by solving the governing PDE.

In this paper, we first consider scattering problems with two radiation channels. For a resonant structure with a nondegenerate resonant mode of complex frequency $\omega_\star$, we derive a simple approximation for the frequency-dependent scattering matrix based on the scat-
tering matrix at \( \omega_0 = \text{Re}(\omega_*) \). The corresponding approximations to the transmission and reflection spectra are accurate for real frequencies near \( \omega_0 \), and predict the peaks and dips in the spectra very well. Moreover, the derived approximate scattering matrix can be used to determine the zeros of the transmission and reflection coefficients, and to reveal the conditions under which the zeros are real. To support and supplement our theory on approximating scattering matrices, we develop a revised TCMT for general scattering problems. The original TCMT gives rise to a symmetric scattering matrix that depends on the scattering matrix \( C \) of the direct passageway \( \tilde{C} \). For scattering problems where the original and reciprocal waves propagate in different radiation channels, the scattering matrix is in general non-symmetric. Our revised TCMT produces a model scattering matrix which is non-symmetric in general, is independent of \( C \), and is consistent with the approximation derived directly.

The rest of the paper is organized as follows. In Sec. II, we recall the definitions and properties of scattering matrices and resonant modes for two-dimensional (2D) structures with a single periodic direction. In Sec. III, we derive approximate formulas for general 2 \( \times \) 2 scattering matrices and related transmission/reflection spectra. In Sec. IV, we present a revised TCMT and derive a simple model for the scattering matrix. For validating our theory, numerical examples involving periodic arrays of cylinders are presented in Sec. V. The paper is concluded with a brief discussion in Sec. VI.

II. PERIODIC STRUCTURES

In this section, we introduce scattering matrices and resonant modes using a two-dimensional (2D) periodic structure as an example. Although the theories developed in the next two sections are applicable to more general cases, they will be validated by numerical examples involving periodic structures. We consider a lossless periodic structure that is invariant in \( z \), periodic in \( y \) with period \( L \), and sandwiched between two identical homogeneous media given for \( x > D \) and \( x < -D \), respectively, where \( \{x, y, z\} \) is a Cartesian coordinate system. The dielectric function \( \varepsilon(x, y) \) of the structure and the surrounding media is real and satisfies

\[
\varepsilon(x, y) = \varepsilon(x, y + L)
\]

for all \( (x, y) \) and \( \varepsilon(x, y) = \varepsilon_0 \geq 1 \) for \(|x| > D\). In particular, the periodic structure may be a periodic array of dielectric cylinders as shown in Fig. I of Sec. V.

For the \( E \) polarization, the \( z \) component of a time-harmonic electric field, denoted by \( u \), satisfies the following 2D Helmholtz equation

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \left( \frac{\omega}{c} \right)^2 \varepsilon(x, y) u = 0,
\]

where the time dependence is \( \exp(-i\omega t) \), \( \omega \) is the angular frequency, \( i \) is the imaginary unit, \( t \) is the time variable, and \( c \) is the speed of light in vacuum. For a real frequency \( \omega \) and a real \( \beta \) satisfying

\[
|\beta| < \frac{\omega}{c}\sqrt{\varepsilon_0} < \frac{2\pi}{L} - |\beta|,
\]

we illuminate the periodic structure by plane waves with wavevectors \((\pm \alpha, \beta)\) from left and right, respectively, where

\[
\alpha = \sqrt{\left(\frac{\omega}{c}\right)^2 \varepsilon_0 - \beta^2}
\]

is positive. The total field in the left homogeneous medium can be written as

\[
u(x, y) = b_1^+ e^{i[\beta y + \alpha(x+D)]} + b_1^- e^{i[\beta y - \alpha(x+D)]} + \sum_{j \neq 0} b_{1j} e^{i[\beta y + \tau_j(x+D)]}, \quad x < -D,
\]

where \( b_1^+ \) is the amplitude of the left incident wave, \( b_1^- \) is the amplitude of the outgoing wave in the left homogeneous medium,

\[
\beta_j = \beta + 2\pi j/L, \quad \tau_j = \sqrt{\beta_j^2 - \left(\frac{\omega}{c}\right)^2 \varepsilon_0}
\]

for \( j \neq 0 \), \( \tau_j \) is positive, and \( b_{1j} \) is the amplitude of the evanescent plane wave \((jth \text{ diffraction order})\) that decays exponentially as \( x \to -\infty \). Similarly, the total field in the right homogeneous medium is given by

\[
u(x, y) = b_2^+ e^{i[\beta y - \alpha(x-D)]} + b_2^- e^{i[\beta y + \alpha(x-D)]} + \sum_{j \neq 0} b_{2j} e^{i[\beta y - \tau_j(x-D)]}, \quad x > D,
\]

where \( b_2^+ \) is the amplitude of the right incident wave, \( b_2^- \) is the amplitude of the right outgoing wave, \( b_{2j} \) is the amplitude of the \( j \)th diffraction order that decays exponentially as \( x \to +\infty \). Since the problem is linear, there is a \( 2 \times 2 \) matrix \( S \), the scattering matrix, such that

\[
\begin{bmatrix}
b_1^- \\
b_2^+
\end{bmatrix} = S \begin{bmatrix}
b_1^+ \\
b_2^-
\end{bmatrix}, \quad S = \begin{bmatrix} r & t \\ \bar{r} & \bar{t} \end{bmatrix}.
\]

In the above, \( r \) and \( t \) (\( \bar{r} \) and \( \bar{t} \)) are the reflection and transmission coefficients respectively, for left (right) incident waves.

It is clear that \( S \) depends on both \( \omega \) and \( \beta \). By analytic continuation, the definition of \( S \) can be extended to the complex \( \omega \) plane. Notice that for a complex \( \omega \), \( \alpha \) and \( \tau_j \) are also complex. Since we assume the structure is lossless (i.e. \( \varepsilon \) is real), the power carried by the incident and outgoing waves must be the same. This implies that for real \( \omega \) and \( \beta \), \( S(\omega, \beta) \) is a unitary matrix. The generalization to complex \( \omega \) is

\[
S(\omega, \beta)S^*(\bar{\omega}, \bar{\beta}) = I
\]

where \( \bar{\omega} \) is the complex conjugate of \( \omega \), \( S^*(\bar{\omega}, \bar{\beta}) \) is the conjugate transpose of \( S \) evaluated at \((\bar{\omega}, \bar{\beta})\), and \( I \) is the identity matrix. A proof for Eq. (9) is given in Ref. [22].
Another important property of $S$ is
\[ S^T(\omega, \beta) = S(\omega, -\beta), \tag{10} \]
where $S^T$ is the transpose of $S$. This is a consequence of the reciprocity and it is valid even when $\omega$ is complex. A proof can be found in Ref. [22]. Notice that, if $\beta \neq 0$, the scattering matrix $S$ is non-symmetric in general.

For periodic structures with a proper symmetry, the scattering matrix can be further simplified [4]. If the structure is symmetric in $y$, i.e., $\varepsilon(x, y) = \varepsilon(x, -y)$, then $S$ is a symmetric and $S$ is a symmetric and $S$ is symmetric in $x$. Moreover, if the periodic structure is symmetric in $x$, i.e., $\varepsilon(x, y) = \varepsilon(-x, y)$, then $\tau = \hat{r}$. More details can be found in Refs. [4] and [22].

Different kinds of eigenmodes can exist in the periodic structure. Due to the periodicity in $y$, any eigenmode is a Bloch mode given by $u(x, y) = e^{i\beta y}\phi(x, y)$, where $\beta \in (-\pi/L, \pi/L]$ is the Bloch wavenumber and $\phi$ is periodic in $y$ with period $L$. Moreover, an eigenmode must satisfy proper boundary conditions as $x \to \pm \infty$. Typically, the wave field should decay exponentially or be outgoing (radiating out power) as $x \to \pm \infty$. In a lossless structure (without material loss), an eigenmode that radiates out power to infinity ($x = \pm \infty$) cannot have both real $\omega$ and real $\beta$. A resonant mode is an eigenmode with a real $\beta$ and a complex $\omega$ satisfying the outgoing radiation condition as $x \to \pm \infty$ [14, 22]. For the assumed time dependence $e^{-i\omega t}$, the imaginary part of $\omega$ is negative, and thus the amplitude of the resonant mode decays with time $t$. If we assume condition [3] is valid with $\omega$ replaced by $\text{Re}(\omega)$, then a resonant mode satisfies
\[ u(x, y) = d_1 e^{i[\beta y - \alpha(x+d)]} + \sum_{j \neq 0} d_{1j} e^{i\beta_j y + \tau_j(x+d)} \tag{11} \]
for $x < -d$ and
\[ u(x, y) = d_2 e^{i[\beta y + \alpha(x-d)]} + \sum_{j \neq 0} d_{2j} e^{i\beta_j y - \tau_j(x-d)} \tag{12} \]
for $x > d$, where $\alpha$ and $\tau_j$ are complex scalars satisfying $\text{Re}(\alpha) < 0$, $\text{Im}(\alpha) < 0$, $\text{Re}(\tau_j) > 0$ and $\text{Im}(\tau_j) > 0$, $d_1$ and $d_2$ are coefficients of the outgoing waves (also called radiation coefficients in this paper), $d_{1j}$ and $d_{2j}$ are coefficients of the evanescent waves. Since $\text{Im}(\alpha) < 0$, the amplitudes of the outgoing waves increase as $|x|$ is increased. It is well known that resonant modes form bands that depend on $\beta$ continuously. Each band corresponds to $\omega$ being a complex-valued function of $\beta$. In the rest of this paper, we denote a resonant mode by $u_\omega$ and its complex frequency by $\omega_\omega$.

If the scattering matrix $S$ is invertible, Eq. [8] can be written as
\[ S^{-1}(\omega, \beta) \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} b_1^* \\ b_2^* \end{bmatrix}. \tag{13} \]
Since the definition of $S$ has been extended to complex $\omega$, the above is also valid for a resonant mode with a complex frequency $\omega_\omega$. Comparing Eqs. [11] and [12] with Eqs. [3] and [10], we obtain
\[ S^{-1}(\omega_\omega, \beta) \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{14} \]
Therefore, $S^{-1}$ is singular at $\omega_\omega$. In other words, $\omega_\omega$ is a pole of $S$. Using Eq. [10], the above can be written as
\[ S^T(\omega_\omega, \beta) \begin{bmatrix} d_1^* \\ d_2^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{15} \]

Due to the reciprocity, corresponding to a resonant mode $u_\omega$ with a real Bloch wavenumber $\beta \neq 0$ and complex frequency $\omega_\omega$, there is always another resonant mode $u'_\omega$ with Bloch wavenumber $-\beta$ and the same complex frequency $\omega_\omega$. Let $d'_1$ and $d'_2$ be the radiation coefficients of $u'_\omega$, then Eq. [14] implies
\[ S^{-1}(\omega_\omega, -\beta) \begin{bmatrix} d'_1 \\ d'_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{16} \]
Taking the complex conjugate of above and using Eqs. [9] and [11], we obtain
\[ S(\overline{\omega_\omega}, \beta) \begin{bmatrix} \overline{d}_1 \\ \overline{d}_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{17} \]

The above means that $\overline{\omega_\omega}$ is zero of the scattering matrix, i.e., for the given $\beta$, $S$ is singular at $\overline{\omega_\omega}$. Notice that since $\varepsilon$ is real, $\overline{\omega_\omega}$ (the complex conjugate of $u'_\omega$) is also a solution of Eq. [2]. In fact, $\overline{\omega}_\omega$ is the time reversal of $u'_\omega$. It has a Bloch wavenumber $\bar{\beta}$, a complex frequency $\overline{\omega_\omega}$, incoming waves with coefficients $\overline{d}_1$ and $\overline{d}_2$, and no outgoing waves. Equation [16] can be directly obtained by applying $S$ to $\overline{\omega}_\omega$.

### III. APPROXIMATE FORMULAS

In this section, we derive approximate formulas for a general $2 \times 2$ scattering matrix and related transmission/reflection spectra, assuming there is a nondegenerate high quality-factor resonant mode with a complex frequency $\omega_\omega = \omega_0 - i\gamma$. The quality factor ($Q$ factor) is given by $Q = \omega_0/(2\gamma)$ and is assumed to be large. The general scattering matrix $S$ depends on the frequency $\omega$ and satisfies Eqs. [9], [15] and [16]. In addition, we assume $\omega_\omega$ is well separated from other resonances, such that in the complex $\omega$ plane, there exists a connected domain $\Omega$ containing $\omega_\omega$, $\overline{\omega}_\omega$, and $\omega_0$, and $\omega_\omega$ is the only pole of $S$ in $\Omega$. The approximate formulas are valid for $\omega$ near $\omega_0$.

Since the resonant mode is nondegenerate, $\omega_\omega$ is a simple pole and $\overline{\omega}_\omega$ is a simple zero of $S$. Therefore,
\[ \det(S) = f(\omega) \frac{\omega - \omega_\omega}{\omega - \overline{\omega}_\omega}, \tag{17} \]
where \( f \) is an analytic function of \( \omega \) on \( \Omega \) and \( f(\omega_*) \neq 0 \). Using Eq. (1), it is easy to show that

\[
\overline{f(\omega)} f(\omega) = 1, \tag{18}
\]

where \( \overline{f(\omega)} \) is the complex conjugate of \( f(\omega) \). Clearly, if \( \omega \) is real, then \( |f(\omega)| = 1 \). The function \( f \) maps \( \Omega \) to \( f(\Omega) = \{ \omega = f(\omega) \mid \omega \in \Omega \} \). If in the complex plane, the exterior of \( f(\Omega) \) contains a ray that goes from the origin to infinity, then it can be used as the branch cut to define a complex square root function, so that \( g(\omega) = \sqrt{f(\omega)} \) is analytic on \( \Omega \). Assuming this is the case, we now rewrite the scattering matrix as

\[
S(\omega) = \begin{bmatrix} r & \tilde{t} \\ t & \tilde{r} \end{bmatrix} = \frac{g(\omega)}{\omega - \omega_*} \begin{bmatrix} R & \tilde{T} \\ T & \tilde{R} \end{bmatrix}, \tag{19}
\]

where \( R, T, \tilde{R} \) and \( \tilde{T} \) are all analytic functions of \( \omega \) on \( \Omega \). Using Eqs. (19) and (17), we can show that

\[
\begin{aligned}
\tilde{R}(\omega) &= \overline{R(\omega)}, \\
\tilde{T}(\omega) &= -\overline{T(\omega)}, \\
R(\omega) \tilde{R}(\omega) - T(\omega) \tilde{T}(\omega) &= (\omega - \omega_*) (\omega - \omega_*^*),
\end{aligned} \tag{20}
\]

At \( \omega_0 \), the scattering matrix is

\[
S(\omega_0) = \begin{bmatrix} r_0 & \tilde{t}_0 \\ t_0 & \tilde{r}_0 \end{bmatrix} = \frac{g(\omega_0)}{\omega_0 - \omega_*} \begin{bmatrix} R_0 & \tilde{T}_0 \\ T_0 & \tilde{R}_0 \end{bmatrix} \tag{22}
\]

where \( r_0 = r(\omega_0), t_0 = t(\omega_0), g_0 = g(\omega_0) \), etc. From Eqs. (21) and (22), we obtain

\[
F_0 = \frac{g_0^2}{\omega_0 - \omega_*} - \det S_0, \quad R_0 = \frac{i \gamma r_0}{g_0}, \quad T_0 = \frac{i \gamma t_0}{g_0}. \tag{23}
\]

We assume \( S_0 \) is given and try to approximate \( S \) for \( \omega \) near \( \omega_0 \). For that purpose, we expand \( R \) and \( T \) in Taylor series at \( \omega_0 \):

\[
\begin{aligned}
R(\omega) &= R_0 + R_1 (\omega - \omega_0) + O \left( (\omega - \omega_0)^2 \right), \\
T(\omega) &= T_0 + T_1 (\omega - \omega_0) + O \left( (\omega - \omega_0)^2 \right),
\end{aligned} \tag{24}
\]

where \( R_1 \) and \( T_1 \) are the derivatives of \( R \) and \( T \) (with respect to \( \omega \)) evaluated at \( \omega_0 \). Since \( \tilde{R} \) and \( \tilde{T} \) satisfy Eq. (20), we have

\[
\begin{aligned}
\tilde{R}(\omega) &= \overline{R(\omega)} = \overline{R_0} + \overline{R_1} (\omega - \omega_0) + O \left( (\omega - \omega_0)^2 \right), \\
\tilde{T}(\omega) &= -\overline{T(\omega)} = -\overline{T_0} - \overline{T_1} (\omega - \omega_0) + O \left( (\omega - \omega_0)^2 \right). \tag{26}
\end{aligned}
\]

We approximate the scattering matrix by

\[
S \approx \frac{g(\omega)}{\omega - \omega_*} \left\{ \frac{R_0}{T_0} - \overline{T_0} \right\} + (\omega - \omega_0) \left\{ \frac{R_1}{T_1} - \overline{T_1} \right\}. \tag{27}
\]

To find \( R_1 \) and \( T_1 \), we use Eq. (15) assuming \( d = [d_1, d_2]^T \) is a given unit vector. Equation (15) can be reduced to

\[
\begin{bmatrix} R(\omega_*) & T(\omega_*) \\ -\tilde{T}(\omega_*) & \tilde{R}(\omega_*) \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{38}
\]

Writing down the above using the expansions of \( R \) and \( T \), we obtain

\[
R_1 \approx \frac{1}{g_0} \left[ \left( |d_2|^2 - |d_1|^2 \right) r_0 - 2 d_1 \overline{d_2} t_0 \right] \tag{28}
\]

\[
T_1 \approx \frac{1}{g_0} \left[ -2 d_1 d_2 r_0 + \left( |d_1|^2 - |d_2|^2 \right) t_0 \right]. \tag{29}
\]

The above can be written as

\[
\begin{bmatrix} R_1 \\ T_1 \end{bmatrix} \approx \frac{1}{g_0} H \begin{bmatrix} r_0 \\ t_0 \end{bmatrix},
\]

where \( H = I - 2dd^* \) is a Hermitian unitary matrix satisfying \( H^* = H^{-1} \). Let \( \rho(\omega) = g_0/g(\omega) \), then the final result is

\[
\rho(\omega) S(\omega) \approx S_0 - 2 \frac{\omega - \omega_0}{\omega - \omega_*} dp^T (I - 2 \frac{\omega - \omega_0}{\omega - \omega_*} dd^*) S_0, \tag{30}
\]

where \( p = S_0^T d \) and \( I \) is the identity matrix.

Equation (30) approximates \( \rho(\omega) S(\omega) \) using the scattering matrix at \( \omega_0 \), the complex frequency \( \omega_* \), and the radiation coefficients \( d \) of the resonant mode. However, it is not an approximation to \( S \), since \( \rho \) is an unknown function related to \( f \). Fortunately, for any real \( \omega \), \( |\rho(\omega)| = 1 \), thus, the reflection and transmission spectra can be approximated precisely. The first column of Eq. (30) gives

\[
\begin{aligned}
|r(\omega)| &= \left| r_0 - 2 \frac{\omega - \omega_0}{\omega - \omega_*} \left( |d_1|^2 r_0 + d_1 \overline{d_2} t_0 \right) \right|, \tag{31}
|t(\omega)| &= \left| t_0 - 2 \frac{\omega - \omega_0}{\omega - \omega_*} \left( \overline{d_1} d_2 r_0 + |d_2|^2 t_0 \right) \right|. \tag{32}
\end{aligned}
\]

Moreover, Eq. (30) allows us to find approximately the zeros of the transmission and reflection coefficients. Let \( \omega_*^r \) and \( \omega_*^t \) be the zeros of \( r(\omega) \) and \( t(\omega) \), respectively. For simplicity, we call \( \omega_*^r \) a reflection zero and \( \omega_*^t \) a transmission zero. From the leading terms in (21) and (26), and assuming \( R_1 \) and \( T_1 \) are nonzero, we get

\[
\omega_*^r \approx \omega_0 - \frac{R_0}{R_1}, \quad \omega_*^t \approx \omega_0 - \frac{T_0}{T_1}. \tag{33}
\]

Using \( R_0, T_0, R_1 \) and \( T_1 \) given in Eqs. (28), (29) and (20), we obtain

\[
\begin{aligned}
\omega_*^r \approx \omega_0 + \frac{i \gamma r_0}{( |d_1|^2 - |d_2|^2 |) r_0 + 2 d_1 \overline{d_2} t_0}, \\
\omega_*^t \approx \omega_0 + \frac{i \gamma t_0}{2 d_1 \overline{d_2} r_0 + ( |d_2|^2 - |d_1|^2 |) t_0}. \tag{34}
\end{aligned}
\]

Apparently, \( \omega_*^r \) and \( \omega_*^t \) are complex in general.

In Sec. II, we mentioned that when the periodic structure has a proper symmetry, the reflection and/or transmission coefficients for the left and right incident waves are identical, and in that case, \( \omega_*^r \) and/or \( \omega_*^t \) are real and/or complex. For the case of equal transmission coefficients, i.e., \( t = t \) for all \( \omega \), the scattering matrix \( S \) is symmetric,
Thus \( T(\omega) = -\overline{T(\omega)} \). This implies that if \( \omega \) is real, then \( T(\omega) \) is pure imaginary, and consequently, \( \omega^+_{\omega} \) and \( \omega^−_{\omega} \) are pure imaginary, and \( \omega^0_{\omega} \) is real. Considering the leading terms in the expansions (24)-(27), we have

\[
\omega_{\omega}^+ = \omega_0 + \frac{\gamma t_0/g_0}{2 \text{Im}(d_1d_2t_0/g_0)}. \tag{35}
\]

The above gives an approximate real zero for the transmission coefficient. Notice that the above formula requires a nonzero \( r_0 \).

For the case of equal reflection coefficients, i.e. \( r = \tilde{r} \) for all \( \omega \), we have \( R(\omega) = \overline{R(\omega)} \). Therefore, \( R(\omega) \) is real for real \( \omega \), and \( R_0 \) and \( R_1 \) are also real. The leading terms in the expansions (24)-(27) give rise to

\[
\begin{align*}
\omega_{\omega}^+ &\approx \omega_0 + \frac{i \gamma r_0/g_0}{2 \text{Re}(d_1d_2t_0)/g_0}, \\
\omega_{\omega}^− &\approx \omega_0 + \frac{i \gamma t_0/g_0}{2 \text{Re}(d_1d_2t_0)/g_0}, \\
\omega_{\omega}^0 &\approx \omega_0 + \frac{i \gamma r_0/g_0}{2 \text{Re}(d_1d_2t_0)/g_0}.
\end{align*}
\tag{36}
\]

and \( \omega_{\omega}^0 \) is real.

For the case with \( t = \tilde{t} \) and \( r = \tilde{r} \), Eq. (15) becomes

\[
\begin{bmatrix}
R(\omega) & T(\omega) \\
T(\omega) & R(\omega)
\end{bmatrix}
\begin{bmatrix}
\tilde{d}_1 \\
\tilde{d}_2
\end{bmatrix}
= \begin{bmatrix}
0 \\
0
\end{bmatrix}.
\]

Since the resonant mode with complex frequency \( \omega_\ast \) is nondegenerate, \( R(\omega) \) and \( T(\omega) \) cannot both be zero. It is also impossible for one of them to be zero, because otherwise, \( d \) would be a zero vector. Therefore, both \( R(\omega) \) and \( T(\omega) \) are nonzero. In that case, \( \tilde{d}_1^2 = \tilde{d}_2^2 \), and we can scale \( d \), such that

\[
d_1 = \pm d_2 = 1/\sqrt{2},
\]

where the plus or minus sign depends on the symmetry of the resonant mode. With the given \( d \), the formulas for \( R_1 \) and \( T_1 \) are simplified to

\[
R_1 \approx \pm \frac{t_0}{g_0}, \quad T_1 \approx \pm \frac{r_0}{g_0}.
\]

Equations (31) and (32) are reduced to

\[
|r(\omega)| \approx \frac{i \gamma r_0 (\omega - \omega_\ast) t_0}{\omega - \omega_\ast}, \tag{37}
\]

\[
|t(\omega)| \approx \frac{i \gamma t_0 (\omega - \omega_\ast) r_0}{\omega - \omega_\ast}. \tag{38}
\]

Assuming both \( r_0 \) and \( t_0 \) are nonzero, we can simplify the expressions for the zeros of the reflection and transmission coefficients as

\[
\omega_{\omega}^+ \approx \omega_0 \pm \frac{i \gamma r_0}{t_0}, \quad \omega_{\omega}^− \approx \omega_0 \pm \frac{i \gamma t_0}{r_0}. \tag{39}
\]

Since \( t_0/g_0 \) is real and \( r_0/g_0 \) is pure imaginary, \( t_0/r_0 \) and \( r_0/t_0 \) are pure imaginary. Therefore, both \( \omega_{\omega}^+ \) and \( \omega_{\omega}^− \) are real.

**IV. COUPLED MODE THEORY**

In a seminal work \[5\], Fan et al. developed a TCMT for a resonator connected with \( m \) ports. Assuming the resonator has a single resonant mode with a complex frequency \( \omega_\ast = \omega_0 - i \gamma \) and there is no material loss in the structure, the TCMT states that

\[
\frac{da}{dt} = -i \omega_\ast a + b^\ast b^+ \tag{40}
\]

\[
b^- = CB^+ + ad \tag{41}
\]

\[
|d|^2 = 2 \gamma \tag{42}
\]

\[
C^* = C^{-1} \tag{43}
\]

\[
p = -C^T \overline{d} \tag{44}
\]

\[
C = C^T \tag{45}
\]

\[
p = d \tag{46}
\]

where \( a = a(t) \) is time-dependent amplitude of the resonant mode scaled such that \( |a|^2 \) is the energy of the resonant mode in the resonator, \( b^+ \) and \( b^- \) are column vectors of \( b_j^+ \) and \( b_j^- \) (for \( j = 1, 2, ..., m \)), respectively, \( b_j^+ = b_j^+(t) \) is the time-dependent amplitude of the incoming wave in the \( j \)th port scaled such that \( |b_j^+|^2 \) is the power of the incoming wave, \( b_j^- \) is similarly defined for the outgoing wave, \( p \) is a column vector of coupling coefficients connecting incoming waves with the resonant mode, \( d \) is a column vector for the radiation coefficients of the resonant mode and it couples the resonant mode to the outgoing waves, \( C \) is the scattering matrix for the direct non-resonant passway. For time harmonic waves, the TCMT gives the following scattering matrix:

\[
S(\omega) = C - \frac{dp^T}{i(\omega - \omega_\ast)}. \tag{47}
\]

The above TCMT for a single-mode resonator is constructed by considering energy conservation, reciprocity and time-reversal symmetry. It is assumed that the
original and reciprocal waves exist in the same resonator/ports structure, and consequently, $C$ and $S$ are required to be symmetric. Since energy must be conserved, the matrix $C$ should be unitary. Additional conditions on $d$ and $p$, including Eq. (42), are obtained when Eqs. (40) and (41) are applied to the resonant mode and its time reversal. These conditions and the symmetry of $S$ give rise to Eq. (40). Equation (41) is obtained when the scattering matrix is applied to the time-reversed resonant mode. The TCMT can be extended to more complicated resonant systems. A TCMT for multimode resonators was developed by Suh et al. [10]. Recently, Zhao et al. [13] developed a new TCMT by considering both the original physical system and the time-reversal conjugate system. The new TCMT establishes the constraints of energy conservation, reciprocity and time-reversal symmetry separately, and it is applicable to a wider range of resonant systems. For reciprocal systems, the scattering matrices $C$ and $S$ are also symmetric in the recent works [17, 18].

The TCMT is applicable to diffraction problems of periodic structures with normal incident plane waves where the ports are the propagating diffraction orders. However, it is not applicable to diffraction problems with oblique incident waves, since in that case the scattering matrix is not symmetric. As we mentioned in Sec. II, when there is a nonzero wavenumber $\beta$ for the periodic direction, the reciprocal wave has a different set of diffraction orders, and the scattering matrix satisfies Eq. (10) and is non-symmetric in general. Furthermore, to apply the TCMT to a specific problem, it is necessary to calculate the complex frequency $\omega_*$ and radiation coefficients $d$, and estimate the scattering matrix $C$. It appears that $C$ cannot be calculated rigorously, because the resonant and non-resonant wave field components cannot be separated easily. For the case of a photonic crystal slab, the matrix $C$ may be approximated by the scattering matrix of a uniform slab, but the refractive index of the uniform slab can only be obtained by data fitting [5, 15].

In the following, we present a revised TCMT where the scattering matrix is non-symmetric in general and $C$ is replaced by the scattering matrix at $\omega_0$. We start with the same Eqs. (10) and (11) for a resonant mode with amplitude $a$ and complex frequency $\omega_*$, incoming/outgoing waves with amplitudes $b_j^\pm$ in the $j$th radiation channel, and a scattering matrix $C$ for the direct non-resonant passway. The scattering matrix given in Eq. (47) remains valid. Since the reciprocal waves propagate in a different set of radiation channels, we have

\[
\frac{db'}{dt} = -i\omega_* b' + p'^Tb^+ \quad (48)
\]

\[
b'^+ = C'b^+ + a'd' \quad (49)
\]

\[
S'(\omega) = C' - \frac{dp'^T}{i(\omega - \omega_*)} \quad (50)
\]

where $a'$ is the amplitude of the reciprocal mode, $b_j^+$ is the amplitude of incoming wave in the $j$th reciprocal radiation channel, $C'$ is the scattering matrix for direct passway in the reciprocal system, $S'$ is the frequency-dependent scattering matrix of the reciprocal system, etc. Notice that Eqs. (48)–(50) are different from those for the time-reversal conjugate system [13].

In view of Eq. (11), the reciprocity principle requires that $C' = C^T$ and $S' = S^T$, and thus

\[
d'p'^T = pd^T. \quad (51)
\]

In addition, the conservation of energy implies that $C$ must be a unitary matrix. Applying the theory to the resonant mode and the reciprocal mode as in Ref. [3], we obtain

\[
||d||^2 = ||d'||^2 = 2\gamma. \quad (52)
\]

Importantly, the time-reversed resonant mode propagates in the reciprocal radiation channels, and satisfies Eqs. (48)–(50), and the time-reversal reciprocal mode satisfies Eqs. (10), (41) and (47). Applying the theory to the time-reversed modes as in Ref. [3], we obtain

\[
p^Td' = p'^Td = 2\gamma, \quad C'd = -d, \quad C'^pd = -d'. \quad (54)
\]

Solving Eqs. (51), (52) and (53), we obtain

\[
p = d', \quad p' = d. \quad (55)
\]

Therefore, $p$ is the vector of radiation coefficients of the reciprocal mode, Eq. (44) is still valid, and

\[
S(\omega) = \left[ I + \frac{dd^*}{i(\omega - \omega_*)} \right] C. \quad (56)
\]

In summary, if the original and reciprocal waves propagate in different radiation channels, then TCMT should use Eqs. (40)–(44). The scattering matrix is given in Eq. (47) or (56). At $\omega = \omega_0$, Eq. (47) becomes

\[
S(\omega) = S_0 = C + \frac{1}{\gamma}dp^T. \quad (57)
\]

Therefore,

\[
S(\omega) = S_0 - \frac{\omega - \omega_0}{\gamma(\omega - \omega_*)}dp^T. \quad (58)
\]

Multiplying $d^*$ to both sides of Eq. (57), we obtain

\[
p^T = d^*S_0. \quad (59)
\]

Using the unit vectors

\[
d = \frac{d}{||d||}, \quad p = \frac{p}{||p||} = S_0d, \quad (60)
\]

we can rewrite the scattering matrix as

\[
S(\omega) = S_0 - 2\frac{\omega - \omega_0}{\omega - \omega_*}dp^T
\]

\[
= \left[ I - 2\frac{\omega - \omega_0}{\omega - \omega_*}dd^* \right] S_0. \quad (61)
\]
It can be easily verified that

\[ S(\omega)S^*(\omega) = I. \]  

(62)

Therefore, if \( \omega \) is real, \( S \) is unitary. Moreover,

\[ S^{-1}(\omega_*)d = S^*(\omega_*)d = S^*_0(I - dd^*)d = 0. \]

Therefore, \( \omega_* \) is a zero of \( S^{-1} \) and a pole of \( S \). Similarly,

\[ S^{-T}(\omega_*)p = \overline{S(\omega_*)}p = (I - dd^*)\overline{S}_0p = 0. \]

Notice that Eq. (61) is similar but not identical to Eq. (60) in Sec. III. The latter is derived from the exact scattering matrix, but it is only valid for the 2 \( \times \) 2 case and it contains an unknown analytic function \( \rho \) satisfying \( \rho(\omega_0) = 1 \). For \( \omega \) near \( \omega_0 \), if we approximate \( \rho(\omega) \) by 1, then Eq. (60) is reduced to Eq. (61). It should be emphasized that Eq. (61) is only a model. Although TCMT follows the most important physical principles, it ignores the coupling caused by the evanescent waves, ignores the frequency dependence of the incoming and outgoing waves and the coupling coefficients, ignores the difference between the actual field in the resonator and the resonant mode, etc. On the other hand, Eqs. (60) and (61) do give the same approximate zeros of the reflection and transmission coefficients, and since \( |\rho(\omega)| = 1 \) for real \( \omega \), they also give the same approximate transmission and reflection spectra.

V. NUMERICAL EXAMPLES

In this section, we present numerical examples to validate the approximate formulas derived in Sec. III. The numerical results are obtained for three periodic arrays of dielectric cylinders shown in Fig. 1. The arrays are periodic in \( y \) with period \( L \) and the cylinders are surrounded by air. The dielectric constants of the cylinders and surrounding air are \( \varepsilon_1 = 10 \) and \( \varepsilon_0 = 1 \), respectively. The cross sections of the cylinders shown in Fig. 1(a) and (b) are equilateral triangles with side length \( L_t \). The radius of the circular cylinders shown in Fig. 1(c) is \( a \). The arrays with triangular cylinders have a reflection symmetry in \( y \) or \( x \). The array with circular cylinders is symmetric in both \( x \) and \( y \).

Resonant modes in the periodic arrays form bands that depend on the real Bloch wavenumber \( \beta \) continuously. For \( \beta = 0.02(2\pi/L) \) and \( L_t = 0.7L \), the periodic array shown in Fig. 1(a) supports a resonant mode with normalized complex frequency \( \omega_4L/(2\pi c) = 0.49092 - 1.51 \times 10^{-4}i \) and radiation coefficients satisfying \( d_1/d_2 = 0.8281 - 0.0696i \). For the real frequency \( \omega_0 = \text{Re}(\omega) \), we solve the Helmholtz equation (2) numerically and obtain the scattering matrix \( S_0 \). The reflection and transmission coefficients \( r_0 \) and \( t_0 \) (for left incident waves) satisfy \( |r_0|^2 = 0.821 \) and \( |t_0|^2 = 0.179 \). In Fig. 2 we show the transmission and reflection spectra for the same \( \beta \) and for \( \omega \) near \( \omega_0 \). The solid blue lines and dashed red lines correspond to results obtained by numerical simulation and the approximate formulas (31) and (32), respectively. The numerical and approximate analytic results agree very well. The transmission coefficient has a real zero \( \omega_7^* \approx 0.49099(2\pi/eL) \). The approximate formula (34) or (35) gives \( \omega_7^* \) with five correct digits. Since the periodic structure has only a reflection symmetry in \( y \), the zero of the reflection coefficient is complex, and the reflection spectrum has a nonzero dip.

For the periodic array shown in Fig. 1(b) with \( L_t = 0.5L \) and \( \beta = 0.02(2\pi/L) \), we found a resonant mode with normalized complex frequency \( \omega_6L/(2\pi c) = 0.63148 - 4.49 \times 10^{-4}i \). This mode is even in \( x \), and thus the radiation coefficients are \( d_1 = d_2 = 1/\sqrt{2} \). At \( \omega_0 \), we found reflection and transmission coefficients satisfying \( |r_0|^2 = 0.892 \) and \( |t_0|^2 = 0.108 \). In Fig. 3 we show transmission and reflection spectra for frequencies near \( \omega_0 \). The numerical results are shown as the solid blue lines, and compared with the analytic approximations shown as the dashed red lines. A very good agreement is achieved. The approximate results
are calculated by the formulas (37) and (38) with “+” replaced by the minus sign. Since the periodic structure is symmetric in \( x \), the transmission and reflection coefficients have real zeros \( \omega^T_0 \approx 0.63133(2\pi c/L) \) and \( \omega^R_0 = 0.63281(2\pi c/L) \), respectively. The approximate formula (39) gives \( \omega^t_0 \) with the same five digits and a real reflection zero \( \omega^r_0 \approx 0.63277(2\pi c/L) \) (with four correct digits after rounding).

In Sec. III, we showed that a proper symmetry and a nonzero value of \( r_0 \) (or \( t_0 \)) are conditions for the existence of a real transmission (or reflection) zero. To illustrate this, we consider the periodic array of circular cylinders shown in Fig. 1(c). It is well-known that a lossless periodic dielectric array can support a variety of bound states in the continuum (BICs) which are special resonant modes with a real frequency and an infinite \( Q \) factor [24–32]. For the cylinder radius \( a = 0.2694L \), the periodic array has a symmetry-protected BIC with wavenumber \( \beta_1 = 0 \) and frequency \( \omega_1 = 0.9297(2\pi c/L) \). The radius \( a \) is chosen so that the transmission coefficient (for \( \beta = 0 \)) at the BIC frequency \( \omega_1 \) is exactly zero. To understand the transmission and reflection spectra for \( \beta \) near \( \beta_1 \), it is necessary to consider \( t \) and \( r \) as functions of two variables \( \omega \) and \( \beta \). In Fig. 3(a) and (b), we show transmittance \( |t|^2 \) and reflectance \( |r|^2 \) as functions of \( \omega \) and \( \beta \), respectively. It is known that \( t \) and \( r \) (as functions of two variables) are discontinuous at \( (\omega_1, \beta_1) \). For this example, although \( t(\omega_1, \beta_1) = 0 \) and \( |r(\omega_1, \beta_1)| = 1 \), there is a function of \( \beta \) namely \( \omega^r_\beta = \omega^r_0(\beta) \), such that \( r(\omega^r_\beta, \beta) = 0 \) and \( |t(\omega^r_\beta, \beta)| = 1 \). Meanwhile, for \( \beta \) near \( \beta_1 = 0 \), there is a resonant mode with a complex frequency \( \omega_* = \omega_*(\beta) \), so that \( \omega_*(\beta_1) = \omega_1 \). It turns out that \( \omega^r_0 \approx \omega_0 = \text{Re}(\omega_*) \) for \( \beta \) near \( \beta_1 = 0 \). Specifically, for \( \beta = 0.01(2\pi/L) \), the normalized complex frequency of the resonant mode is \( \omega_* L/(2\pi c) = 0.92965 - 2.1 \times 10^{-5}i \). The reflection coefficient \( r_0 = r(\omega_0, \beta) \) satisfies \( |r_0|^2 = 5.9 \times 10^{-7} \) and it is close to zero. Therefore, the formula for \( \omega^r_0 \) in Eq. (39) breaks down, and there is no real transmission zero near \( \omega_0 \). In Fig. 3(c) and (d), we show the transmission and reflection spectra for \( \beta = 0.01(2\pi/L) \). The transmission spectrum has a Lorentzian line shape with a 100\% peak, and it does not reach zero. The reflection spectrum has a zero dip at \( \omega^r_0 \approx \omega_0 \). The solid lines shown in Fig. 3 are the numerical results. Analytic results based on Eqs. (37) and (38) are shown as the dashed red lines, and they agree with the numerical results very well. Since the resonant mode is even in \( x \), the “+” signs in Eqs. (37) and (38) are replaced by the minus sign.

**VI. CONCLUSION**

For structures with a high-\( Q \) resonant mode, wave scattering exhibits interesting resonance phenomena with sharp peaks and/or dips in transmission, reflection, and other spectra. Analytic studies or models are useful, because numerical solutions are expensive to obtain and do not provide much physical insight. For scattering problems with two radiation channels and assuming the existence of a nondegenerate high-\( Q \) resonant mode sufficiently separated from other resonances, we derived approximate formulas (for the scattering matrix and transmission/reflection spectra) directly from the exact scattering matrix. Unlike the existing model of Popov et al. [4], we do not need to solve the governing PDE to find the zeros of the transmission/reflection coefficients. In fact, our approximate formulas predict the transmission and reflection zeros, whether they are real or complex.

Constructed from a few basic physical principles, the TCMT of Fan et al. [5] gives a symmetric scattering-matrix model that depends on the scattering matrix \( C \) for the direct non-resonant passway. The model is simple and elegant, but \( C \) cannot be calculated rigorously.
We revised the TCMT to scattering problems with (in general) non-symmetric scattering matrices and replaced $C$ by the scattering matrix $S_0$ at the (real) resonant frequency. The revised TCMT and the theory based on direct derivation lead to slightly different approximations to the scattering matrix, but they give exactly the same transmission and reflection spectra. The directly derived results are rigorous, can be further improved if more terms in the Taylor series (24) and (25) are included, but they are restricted to $2 \times 2$ scattering matrices. It is worthwhile to further extend the theories developed in this paper, for example, to problems with a few interacting and possibly degenerate resonant modes.

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