Temporal Coupled-Mode Theory and the Presence of Non-Orthogonal Modes in Lossless Multimode Cavities

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***Abstract*—We develop a general temporal coupled-mode theory for multimode optical resonators. This theory incorporates a formal description of a direct transmission pathway, and is therefore capable of describing Fano interference phenomena in multimode cavities. Using this theory, we prove a general criterion that governs the existence of nonorthogonal modes. The presence of nonorthogonal modes creates interesting transport properties which can not be obtained in normal resonator systems. We validate our theory by comparing its predictions with first-principles finite-difference time-domain simulations and obtaining excellent agreement between the two.**

***Index Terms*—Electromagnetic coupling, filters, optical modulation, optical switches, resonance.**

I. Introduction

THE MODE of a resonator structure is typically defined as the eigenmode of its time-evolution operator [1], [2]. In a closed cavity when both gain and loss are absent, the time-evolution operator is unitary, and the eigenmode of the cavity forms an orthogonal basis. Such an orthogonal basis is commonly used as a starting point for either coupled-mode theory [1], or as the basis for quantization in quantum electrodyanamics. In the presence of cavity gain or loss, the time-evolution operator is no longer unitary in general. Consequently, the resonator eigenmodes may no longer be orthogonal but rather may form a bi-orthogonal basis [2]. For laser cavities where gain is present, the presence of nonorthogonal modes leads to the Petermann excess noise factor that have been extensively studied both theoretically and experimentally in the past decade [3]–[6].

In addition to the use of optical resonator structure as a laser cavity, high quality factor resonances have also been commonly used in filters for many optical information processing applications. In these applications, the optical resonator is typically coupled with several input/output ports to allow frequency-selective energy transfer between the ports, and the spectral lineshapes of the energy transfer are of critical interests. When the material loss inside the optical resonator can be neglected, the overall multiport system, as shown in Fig. 1, is lossless, and can be described in terms of a unitary S-matrix that relates the amplitudes between the output waves and input waves in all the ports. When only a single optical mode is present in the cavity, the S-matrix can be readily calculated using standard temporal coupled mode theory, which relates the amplitudes in the input and output ports to the amplitudes of the mode inside the cavity [7]. In the case where more than one optical mode are present, however, since the cavity by itself couples to the ports and is therefore an open cavity structure, there is a possibility that the optical modes inside the cavity can only be described in terms of nonorthogonal basis functions. The presence of such nonorthogonality should strongly affect the possible forms of the S-matrix, and the transmission and reflection spectra of the overall system. To the best of our knowledge, however, a formalism that allows one to calculate the transmission and reflection properties of a multimode cavity that supports nonorthogonal modes have never been proposed and studied in details.

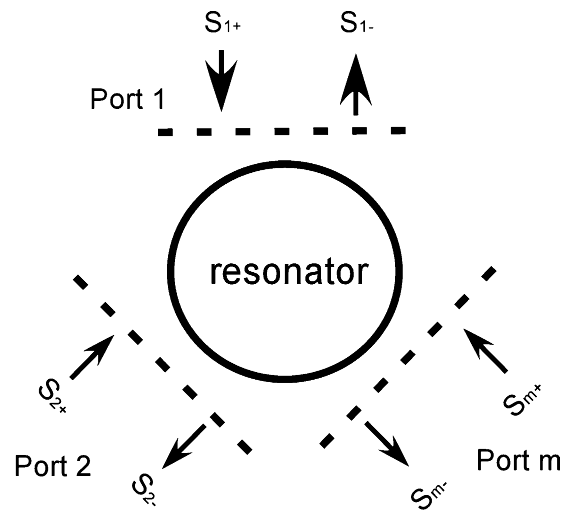

Fig. 1. Schematic of an optical resonator system coupled with multiple ports. The arrows indicate the incoming and outgoing waves. The dashed lines are reference planes for the phase of wave amplitudes in the ports.

In this paper, we develop a general temporal coupled mode theory of a multimode optical resonator. This theory incorporates a formal description of a direct transmission pathway and is therefore capable of describing Fano interference [8]–[10] for the multimode cavity system. Using this theory, we prove a general criterion that governs the existence of nonorthogonal modes in the cavity. In a simple case where only two-modes are present, we provide a detailed derivation of the spectral lineshapes that

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are associated with nonorthogonal modes. We compare the predictions of these lineshapes with first-principle finite-difference time-domain (FDTD) simulations in photonic crystal structures and show that the theoretical prediction indeed produces the correct lineshapes as seen in the simulation. Both theory and simulations indicate that in the presence of nonorthogonal modes, it is possible to generate very sharp transmission peaks even which can potentially be of importance for switching or sensing applications.

The paper is organized as follows. In Section II, we present a detailed derivation for the general coupled mode theory applicable to a system with arbitrary number of ports and resonances. In Section III, we then apply the theory to a two-mode, two-port system to highlight the essential differences in the transport properties between the orthogonal and the nonorthogonal systems. And finally, in Section IV, we present first principles FDTD simulations which completely validate our theoretical analysis.

II. Theory

A. General Discussions and Summary of the Main Results

We develop our theory based upon the coupling of modes in a time-dependent formalism for optical resonators [7]. As a starting point, we consider a closed optical cavity system that possesses n modes coupling with each other. The dynamic equations for resonance amplitudes can be written in the following form:

$$\frac{d\mathbf{a}}{dt} = j\Omega\mathbf{a} \tag{1}$$

where Ω is a $n \times n$ matrix which represents resonance frequencies and the coupling between modes. In general, the cavity modes are coupled and the amount of coupling is determined by the overlap integral of the modes, which determines the off-diagonal elements of Ω. The amplitude vector

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

represents the resonance amplitudes inside the optical cavity. Here the resonance amplitudes are normalized such that $|a_i|^2$ corresponds to the energy in the ith optical mode of the resonator. When there is no gain or loss in the closed system, the energy is conserved. The Ω matrix is therefore Hermitian and can be diagonalized by unitary transformations. The eigenmodes of the Ω matrix form an orthogonal basis. Now, let us imagine that we couple the n-mode resonator system as described by (1), to m ports (Fig. 1). The incoming wave from the ports can then couple into the resonator. At the same time, the amplitude inside the resonator can also decay into the ports. For such a system, the dynamic equations in general can be written as [11]

$$\frac{d\mathbf{a}}{dt} = (j\Omega - \Gamma)\mathbf{a} + K^{\mathrm{T}}|s_+\rangle \tag{2}$$

$$|s_-\rangle = C|s_+\rangle + D\mathbf{a} \tag{3}$$

where both Ω and Γ matrices are $n \times n$ Hermitian matrices, and represent the resonance frequencies and the decay, respectively. The resonant mode is excited by the incoming waves

$$|s_+\rangle = \begin{pmatrix} s_{1+} \\ s_{2+} \\ \vdots \\ s_{\mathrm{m}+} \end{pmatrix}$$

from ports 1 to m, with the coupling matrix

$$K^{\mathrm{T}} = \begin{bmatrix} k_{11} & k_{12} & \cdots & k_{1n} \\ k_{21} & k_{22} & \cdots & k_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ k_{m1} & k_{m2} & \dots & k_{mn} \end{bmatrix}^{\mathrm{T}}.$$

The resonant mode, once excited, coupled with the outgoing waves

$$|s_-\rangle = \begin{pmatrix} s_{1-} \\ s_{2-} \\ \vdots \\ s_{m-} \end{pmatrix}$$

at the ports with the coupling matrix

$$D = \begin{bmatrix} d_{11} & d_{12} & \cdots & d_{1n} \\ d_{21} & d_{22} & \cdots & d_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ d_{m1} & d_{m2} & \dots & d_{mn} \end{bmatrix}.$$

Here we assume that all n eigenvalues of the matrix $j\Omega - \Gamma$ have negative real parts. Thus, all the resonance in the cavity can decay into the ports. (Those modes that do not couple into the ports obviously do not contribute to the resonant transport process. While this might appear to be a trivial statement, we will explicitly use this assumption in the later part of the paper.) In addition to the resonance-assisted coupling between the ports, the incoming and outgoing waves in the ports can also couple through a direct pathway, as described by an $m \times m$ scattering matrix C. The incorporation of such scattering matrix C leads to Fano interference [11].

In general, for any lossless and reciprocal system, the only constraint on matrix C is that it is unitary and symmetric. On the other hand, since the overall system, including both the resonance and the ports, is energy conserving, the decay process, as described by the matrix Γ, results from the coupling of the resonance to the ports. Thus, the matrices K and D should not be independent but rather should be related to Γ and C. In Sections II-B–II-E, we will prove the following relations rigorously:

$$D^{+}D = 2\Gamma \tag{4}$$

$$K = D \tag{5}$$

$$CD^{*} = -D. \tag{6}$$

The proof is completely general and relies upon only time-reversal symmetry and energy conservation arguments.

The multimode temporal coupled mode theory as outlined above should be useful in studying wide ranges of effects in optical resonator systems. Here, in particular, using this theory, we will prove in Section II-F that the resonant modes become

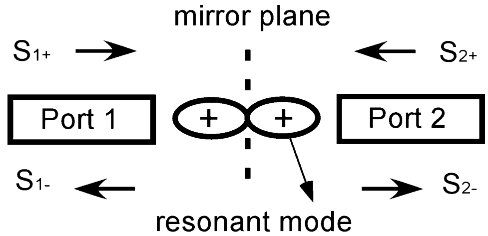

Fig. 2. Schematic of an optical resonator system coupled with two physical ports. The system possesses a mirror plane as represented by the dashed line. Both the system and the resonator mode have even symmetry with respect to the mirror plane.

nonorthogonal when $\mathrm{rank}(j\Omega-\Gamma) > \mathrm{rank}(D)$. And therefore, the presence of nonorthogonal modes is in fact of very general nature in multimode optical resonator systems.

B. Proof of (4): $D^+D = 2\Gamma$

Equation (4) is a direct consequence of energy conservation. To see this, we consider the scenario where the external incident wave is absent, i.e., $|s_+\rangle = 0$, and at $t = 0$, there is a finite amplitude in the resonance. At $t > 0$, the resonant mode will decay exponentially into all the ports, and the energy of the optical modes in the resonator thus varies as

$$\begin{aligned}\frac{d(\mathbf{a}^+\mathbf{a})}{dt} &= \frac{d\mathbf{a}^+}{dt}\mathbf{a} + \mathbf{a}^+\frac{d\mathbf{a}}{dt}\\ &= \mathbf{a}^+(-j\Omega^+ - \Gamma^+)\mathbf{a} + \mathbf{a}^+(j\Omega-\Gamma)\mathbf{a}\\ &= -2\mathbf{a}^+\Gamma\mathbf{a}\end{aligned} \tag{7}$$

where we use the fact that both Ω and Γ are Hermitian matrices. (For clarity, we note that $\mathbf{a}^+$ is the Hermitian adjoint of the resonance amplitude $\mathbf{a}$.) On the other hand, since the overall system, including both the resonator and the ports, is energy conserving, the decaying of the resonance amplitudes are due entirely to the creation of the outgoing waves. Hence

$$\frac{d(\mathbf{a}^+\mathbf{a})}{dt} = -\langle s_-|s_-\rangle = -\mathbf{a}^+D^+D\mathbf{a}. \tag{8}$$

Comparing (7) and (8), we have

$$D^+D = 2\Gamma. \tag{4}$$

C. Concept of Independent Decay Ports

For the proof of (5) and (6), and for the discussions of the presence of nonorthogonal modes, the concept of independent decay ports are of essential importance. We will introduce this concept first with a simple example. Consider a single resonance coupling with two physical ports, as shown in Fig. 2. We assume that the system has a mirror-plane symmetry, and that the resonant mode is even with respect to the mirror plane. The decay amplitudes from the resonance into the two ports are then always equal. In other words, while two physical ports are present, the decay amplitudes in these ports are correlated and are not independent from each other due to the properties of the resonances, and therefore are effectively identical ports. The concept of independent ports is introduced to precisely describe such correlation effects between different physical ports.

In general, we define the number of independent decay ports l as

$$l \equiv \mathrm{rank}(D). \tag{9}$$

Since D is an $m \times n$ matrix, l is always no greater than the number of resonances n and the number of ports m [12]. Furthermore, using singular value decomposition (SVD), we can represent D as [12]

$$D = U\begin{bmatrix}\tilde{D} & 0\\ 0 & 0\end{bmatrix}V^+. \tag{10}$$

Here, U and V are $m \times m$ and $n \times n$ unitary matrices respectively. $\tilde{D}$ is an $l \times l$ diagonal matrix. With the transformation of (10), (3) can be rewritten as

$$|\tilde{s_-}\rangle = \tilde{C}|\tilde{s_+}\rangle + \begin{bmatrix}\tilde{D} & 0\\ 0 & 0\end{bmatrix}\tilde{\mathbf{a}} \tag{11}$$

where $|\tilde{s_+}\rangle = U^+|s_+\rangle$, $|\tilde{s_-}\rangle = U^+|s_-\rangle$, $\tilde{C} = U^+CU$ and $\tilde{\mathbf{a}} = V^+\mathbf{a}$. If we define $|\tilde{s_+}\rangle = \begin{bmatrix}|\tilde{s_+}\rangle_u\\ |\tilde{s_+}\rangle_d\end{bmatrix}$, and $|\tilde{s_-}\rangle = \begin{bmatrix}|\tilde{s_-}\rangle_u\\ |\tilde{s_-}\rangle_d\end{bmatrix}$, we can see from (11) that the outgoing amplitudes $|\tilde{s_-}\rangle_d$ do not come from the resonances. Therefore, from time reversal symmetry, the incoming wave amplitudes $|\tilde{s_+}\rangle_d$ should not couple to the resonances either. Under the same transformations of U and V, the K matrix should become

$$K^{\mathrm{T}} = V^*\begin{bmatrix}\tilde{K}^{\mathrm{T}} & 0\\ 0 & 0\end{bmatrix}U^{\mathrm{T}} \tag{12}$$

where $\tilde{K}^{\mathrm{T}}$ is an $l \times l$ matrix. The use of the concept of independent ports thus reduces the complexity of the temporal coupled mode theory.

D. Proof of (5): $K = D$

Using the concept of independent ports, we now set out to prove (5), with time-reversal symmetry arguments. Let's perform a time-reversal transformation for the exponential decay process as described by (7). The time-reversed case is represented by feeding the resonator with exponentially growing waves at complex frequencies $\omega = \Omega - j\Gamma$, with amplitudes at $t = 0$ equal to $|s_-\rangle^*$. Such excitations cause time reversed resonance amplitudes $\mathbf{a}^*$ at $t = 0$ to grow exponentially in time. From (2), under a steady-state excitation with the frequencies ω, the amplitude of the resonant mode is

$$(j\omega I - j\Omega + \Gamma)\mathbf{a} = K^{\mathrm{T}}|s_+\rangle. \tag{13}$$

Thus, at the complex frequencies $\omega = \Omega - j\Gamma$, we have $2\Gamma^*\mathbf{a}^* = K^{\mathrm{T}}|s_-\rangle^* = K^{\mathrm{T}}(D^*\mathbf{a}^*)$, and therefore

$$K^{\mathrm{T}}D^* = 2\Gamma^*. \tag{14}$$

Using (10) and (12), (14) can be simplified into

$$\begin{bmatrix}\tilde{D}^+\tilde{K} & 0\\ 0 & 0\end{bmatrix} = \begin{bmatrix}2\tilde{\Gamma} & 0\\ 0 & 0\end{bmatrix} \tag{15}$$

where $\tilde{\Gamma}$ is an $l \times l$ Hermitian matrix.

On the other hand, recalling (4): $D^+D = 2\Gamma$, and applying (10) to (4), we have

$$\begin{bmatrix}\tilde{D}^+\tilde{D} & 0\\ 0 & 0\end{bmatrix} = \begin{bmatrix}2\tilde{\Gamma} & 0\\ 0 & 0\end{bmatrix}. \tag{16}$$

Therefore, comparing (15) and (16), we have $\tilde{D}^+(\tilde{D}-\tilde{K})=0$. And immediately $\tilde{K}=\tilde{D}$ follows, since $\tilde{D}^+$ is an $l\times l$ nonsingular matrix. Hence

$$K = U\begin{bmatrix}\tilde{K} & 0\\ 0 & 0\end{bmatrix}V^+ = U\begin{bmatrix}\tilde{D} & 0\\ 0 & 0\end{bmatrix}V^+ = D \tag{17}$$

which proves (5). We note that this result can also be proved using reciprocity.

E. Proof of (6): $CD^* = -D$

The time-reversed excitation $|s_-\rangle^*$ also has to satisfy the condition that no outgoing wave shall occur upon such excitations [11], i.e.,

$$0 = C|s_-\rangle^* + D\mathbf{a}^* = CD^*\mathbf{a}^* + D\mathbf{a}^*. \tag{18}$$

Thus, the coupling constants D have to satisfy a further condition

$$CD^* = -D. \tag{6}$$

Hence, the coupling constants in general cannot be arbitrary, but are instead related to the scattering matrix of the direct process.

F. Condition for the Existence of Nonorthogonal Modes

As an application of the temporal coupled mode theory outlined above, here we show that in an optical resonator system, nonorthogonal modes will always exist when the number of independent decay ports $l=\mathrm{rank}(D)$ is less than the number of leaky optical modes. Recall that the modes of the resonator are defined as the eigenmodes of the operator $H\equiv(j\Omega-\Gamma)$. It is known that the eigenmodes of a matrix H form an orthogonal basis if and only if $H^+H = HH^+$ [12]. Since Ω and Γ are Hermitian, $H^+H=HH^+$ is equivalent to the relation $\Omega\Gamma=\Gamma\Omega$, which implies that Ω and Γ can be simultaneously diagonalized. On the other hand, since $\Gamma=D^+D/2$, we have $\mathrm{rank}(\Gamma)=\mathrm{rank}(D)$. Consequently, when the relations $\Omega\Gamma=\Gamma\Omega$ and $\mathrm{rank}(D)<n$ are both satisfied, some of the eigenmodes of the matrix H will have pure imaginary eigenvalues, which indicates that some modes have infinite lifetime, and do not couple to the ports. This contradicts our initial assumptions on H that all eigenmodes of H should decay into the ports. Therefore, the modes in a resonator system will always be nonorthogonal when the total number of independent decay ports is less than the number of optical modes.

III. Example: A Spatially Symmetric System With Two Modes and Two Ports

In order to highlight the fundamental differences in transport properties between systems with orthogonal or nonorthogonal resonant modes, we study a resonator system with two resonances and two physical ports, as an example of the general theory. Such a system is described by matrices

$$\Omega = \begin{bmatrix}\omega_1 & 0\\ 0 & \omega_2\end{bmatrix}$$

$$\Gamma = \begin{bmatrix}\gamma_1 & \gamma_o\\ \gamma_o^* & \gamma_2\end{bmatrix}$$

$$C = \begin{bmatrix}r_d & t_d\\ t_d & r_d\end{bmatrix}$$

and

$$D = \begin{bmatrix}d_{11} & d_{12}\\ d_{21} & d_{22}\end{bmatrix}.$$

We determine both the D matrix and the off-diagonal elements of the Γ matrix in terms of the resonance frequencies ω_1,ω_2 and the decay rates γ_1 and γ_2, and subsequently obtain the transport characteristics. Applying (4) and (6) to these matrices, and assuming the system has mirror symmetry, we get

$$|d_{11}| = |d_{21}| = \sqrt{\gamma_1} \tag{19}$$

$$|d_{12}| = |d_{22}| = \sqrt{\gamma_2} \tag{20}$$

$$\exp(j\theta_{12}-j\theta_{11}) + \exp(j\theta_{22}-j\theta_{21}) = 2\frac{\gamma_o}{\sqrt{\gamma_1\gamma_2}} \tag{21}$$

where θ_{ij} is the phase angle of d_{ij}. Since the system has mirror plane symmetry, each mode will decay either symmetrically or anti-symmetrically into the two ports, and we have

$$\theta_{1j} = \theta_{2j} + 2n\pi \quad \text{or} \quad \theta_{1j} = \theta_{2j} + (2n+1)\pi. \tag{22}$$

Thus, in general, we obtain

$$\exp(j\theta_{12}-j\theta_{11}) = \pm\exp(j\theta_{22}-j\theta_{21}). \tag{23}$$

Using these equations, we now consider two cases where the resonator modes are of different symmetry properties.

Case (1): The Two Resonances Have Opposite Symmetry: In this case, since the two resonances have opposite symmetry, we have

$$\exp(j\theta_{12}-j\theta_{11}) = -\exp(j\theta_{22}-j\theta_{21}) \tag{24}$$

and from (21) we have $\gamma_o=0$ [13], and therefore the modes are orthogonal ($\Omega\Gamma=\Gamma\Omega$). The transmission through such a system can then be directly determined by theory as

$$t = t_d \mp \frac{\gamma_1(r_d\pm t_d)}{(j\omega - j\omega_1+\gamma_1)} \pm \frac{\gamma_2(r_d\mp t_d)}{(j\omega-j\omega_2+\gamma_2)} \tag{25}$$

where the top signs are used when the first mode is even, and the bottom signs are used when the first mode is odd.

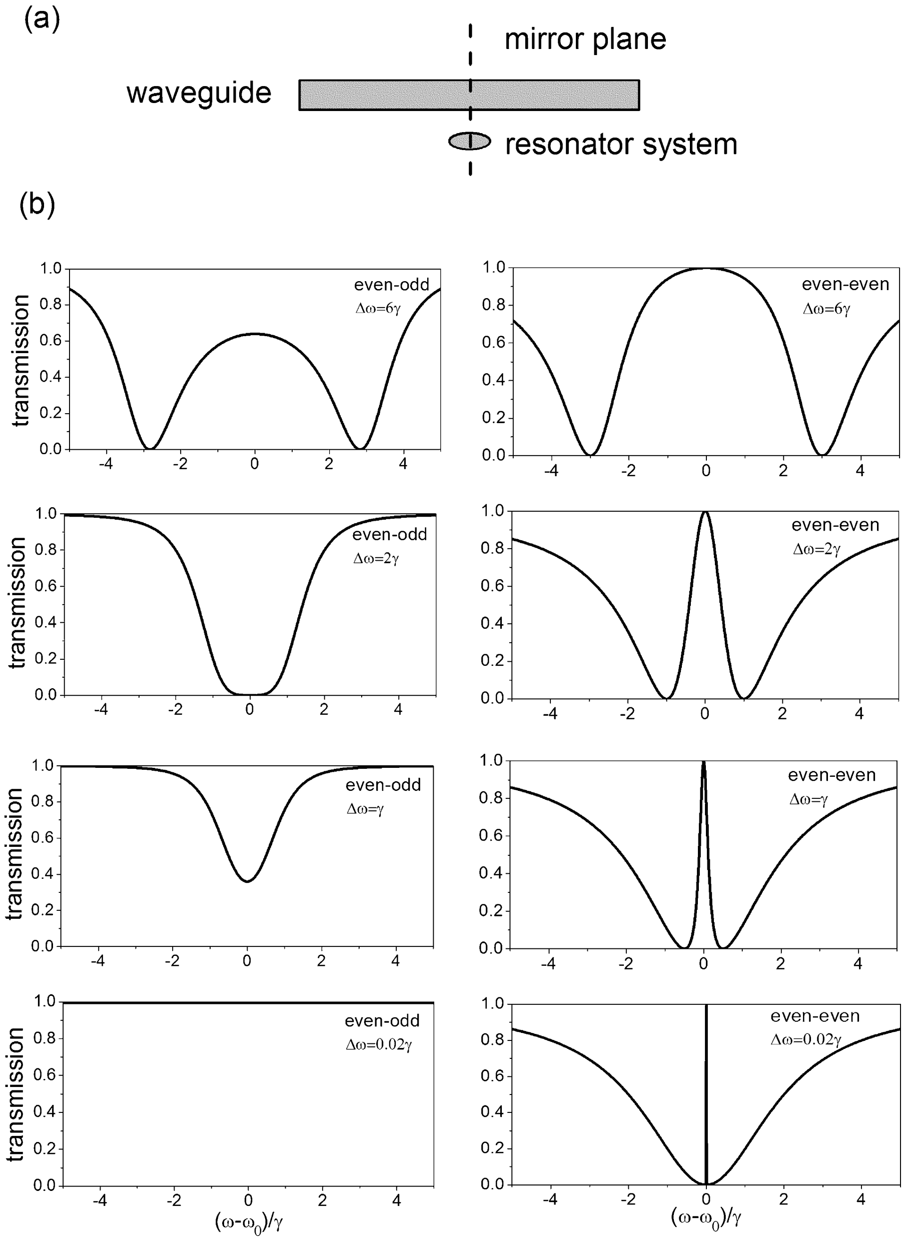

Fig. 3. (a) Schematic of a waveguide side-coupled to an optical resonator system. The resonator system supports two modes. (b) Theoretical transmission spectrum through the system shown in (a). Left panels are when the resonator supports orthogonal modes and right panels are when it supports nonorthogonal modes. We vary the frequency spacing $\Delta\omega$ between the two resonance frequencies. The width of both resonances are assumed to be γ, and ω_0 is the average of the two resonance frequencies.

Case (2). The Two Resonances Have the Same Symmetry: In this case, since the symmetry of the two resonances are the same, the decay amplitudes in the two ports are always equal to each other, and we have only a single independent decay port. From our general arguments in Section II-F, the system should possess nonorthogonal resonant modes.

Mathematically, from (6) and (22), one can show that $[\exp(j2\theta_{i1})] = [\exp(j2\theta_{i2})] = -(r_d + t_d)$ when both modes are even, and $[\exp(j2\theta_{i1})] = [\exp(j2\theta_{i2})] = r_d - t_d$ when both modes are odd. Furthermore, since the scattering matrix C is unitary, in general, we have $r_d r_d^* + t_d t_d^* = 1$, $r_d t_d^* + t_d r_d^* = 0$ and, therefore, $|r_d + t_d| = |r_d - t_d| = 1$. Consequently

$$\exp(j\theta_{12} - j\theta_{11}) = \exp(j\theta_{22} - j\theta_{21}) = \pm 1 \qquad (26)$$

and from (21), we have

$$\gamma_o = \pm\sqrt{\gamma_1\gamma_2}. \qquad (27)$$

Therefore, the resonant modes indeed form a nonorthogonal basis, since $\Omega\Gamma \neq \Gamma\Omega$. The transmission coefficient can be determined as

$$t = t_d \mp \frac{(r_d \pm t_d)\,[\gamma_1(j\omega - j\omega_2) + \gamma_2(j\omega - j\omega_1)]}{(j\omega - j\omega_1 + \gamma_1)(j\omega - j\omega_2 + \gamma_2) - \gamma_1\gamma_2} \qquad (28)$$

where the top signs are used when both modes are even, and the bottom signs are used when both modes are odd.

Fig. 3 shows the transmission through the system with either orthogonal or nonorthogonal modes, as determined using (25) and (28). The system can be realized by a waveguide side coupled to a resonator system, as schematically shown in Fig. 3(a).

We assume that $\omega_1 = \omega_0 - \Delta\omega/2$ and $\omega_2 = \omega_0 + \Delta\omega/2$. For simplicity, we also assume that the two resonances possess the same linewidth γ, and that $t_d = 1$ and $r_d = 0$. And we vary the separation of the resonance frequencies $\Delta\omega$. In the case of orthogonal mode [Fig. 3(b), left panels], when $\Delta\omega \gg \gamma$, the transmission behaves as two separate Lorentzian lineshapes, with high transmission at $\omega = \omega_0$ and with the transmission dropping to zero near ω_1 and ω_2. As the resonance frequencies become closer to each other, the transmission coefficient at $\omega = \omega_0$ starts to decrease, eventually reaching zero when $\Delta\omega = 2\gamma$. In such a case, the lineshape exhibits a flat-top reflection spectrum and the system can be used as a filter to completely reflect a particular wavelength channel while letting other channels pass through [14]. As we further decrease $\Delta\omega$ such that $\Delta\omega < 2\gamma$, the transmission at $\omega = \omega_0$ starts to increase, eventually exhibiting an all-pass transmission characteristic when $\Delta\omega \approx 0$. In such a case, there is significant delay at resonance, while the intensity maintains 100% transmission both on and off resonance. Such a system can be used for optical delay lines [14], [15].

In the case of nonorthogonal mode [Fig. 3(b), right panels], the transmission behavior is significantly different. At the resonance frequencies ω_1 and ω_2, the transmission goes to zero regardless of the spacing between the two resonance frequencies. Furthermore, when the linewidths of the two resonances are same, the transmission peaks at $\omega = \omega_0$ with 100% intensity. (The frequency of this transmission peak, in general, is dependent upon the linewidth of the resonance when the linewidths are not equal, but always occur between the two resonance frequencies.) The width of such transmission peak is dependent upon the frequency spacing of the two modes and can be infinitesimal when the two frequencies are close to each other. Thus, we can achieve narrow-bandwidth behavior in the transmission, where the bandwidth can be tuned by changing the relative position of the resonance frequencies. This could be potentially important for optical switching and sensing applications.

IV. Numerical Validation of the Theory

To validate the theoretical analysis, we compare the theoretical results derived in Section III to FDTD simulations of passive photonic crystal systems with two resonant modes. An example of a system that possesses orthogonal modes is shown in Fig. 4. The crystal consists of a square lattice of dielectric rods. In the crystal, a waveguide is introduced by removing one row of dielectric rods. Also, two identical single-mode cavities are created on the *same side* of the waveguide by reducing the radius of two rods. Since there is a mirror plane symmetry, the overall resonator system possesses even and odd modes, each of which can be approximated as a linear superposition of the two modes in the single-mode cavities. Thus, the two resonator modes are orthogonal. The simulation results as reported previously indeed show excellent agreements with the analytic theory using orthogonal modes. In particular, all-pass transmission characteristics has been observed [15].

Here, we focus our attention on the case of nonorthogonal modes. We again consider a photonic crystal waveguide structure with a square lattice of dielectric rods. The dielectric constant of the rods is 11.56, and the rods have radii of $0.2a$, where

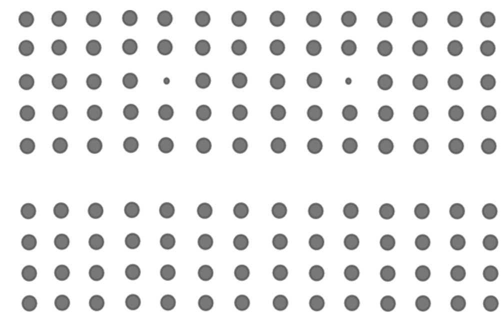

Fig. 4. Schematic of a two-dimensional photonic crystal structure. The gray circles correspond to dielectric rods. The crystal consists of a square lattice of dielectric rods of radius $0.2a$, where a is the lattice constant, with dielectric constant of 11.56. A waveguide is formed by removing one row of dielectric rods. On the same side of the waveguide, there are two identical single-mode cavities of radius $0.05a$ and dielectric constant 4.2. This system is described in terms of an orthogonal mode model.

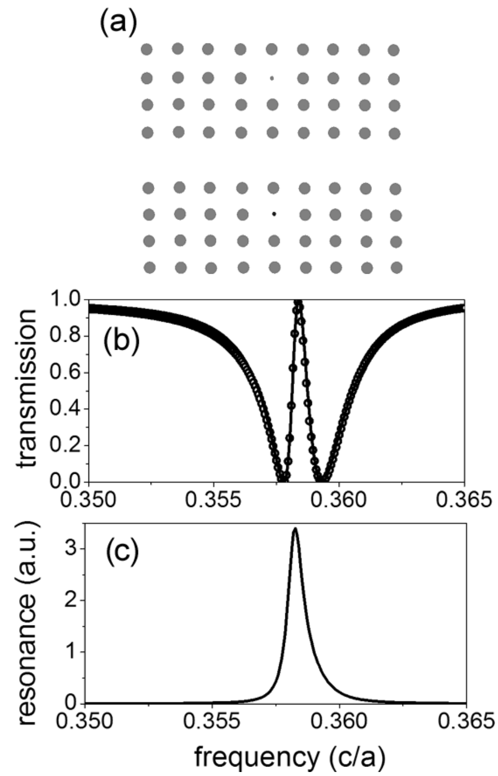

Fig. 5. (a) Schematic of a two-dimensional photonic crystal structure with dielectric rods of radius $0.2a$ and dielectric constant 11.56. A waveguide is formed by removing one row of dielectric rods. One resonator is formed by reducing the radius of a rod three periods from the waveguide to $0.05a$. The second dielectric rod resonator is placed on the opposite side of the waveguide two periods away, by replacing the rod with a rod of radius $0.05a$ and dielectric constant 12.4. This system is described in terms of a nonorthogonal mode model, since both modes have even symmetry with respect to the mirror plane perpendicular to the waveguide. (b) Transmission spectrum through the waveguide structure. Solid line is the analytic theory and the open circles are FDTD simulations. (c) Resonance amplitudes of the two resonances. Note that the two resonances are not distinguishable since the frequency difference is smaller than the resonance linewidth.

a is the lattice constant. We put two single-mode cavities on the *opposite* side of the waveguide as shown in Fig. 5(a). One cavity is formed by reducing the radius of a rod located at three periods from the waveguide to $0.05a$. The second cavity is created by replacing a rod at two periods away from the waveguide, with a rod of radius $0.05a$ and dielectric constant 12.4. Each of the two point defects is chosen to support a monopole mode [16], and thus both modes possess an even field pattern with respect to the mirror plane, in consistency with *case (2)* described in the previous section. Since the number of independent decay ports is less than the total number of leaky resonance, the modes are nonorthogonal. In the simulation, the cavity modes are excited with a temporal Gaussian pulse entering from the left side of the waveguide, and we record the transmission function response at the right end of the waveguide and the amplitudes in the cavities. The transmission spectrum is shown in Fig. 5(b), which clearly shows zero intensity at two frequencies, and a peak that reaches 100%, between these two frequencies. To compare the FDTD results to the analytic theory, we extract the resonance frequencies and the width of the optical modes by analyzing the temporal decaying tail of the resonant modes after the pulse has passed through. The spectrum of resonance amplitudes are shown in Fig. 5(c). In the figure, only a single peak is present, since the frequency difference between the two resonances is smaller than the resonance linewidth. However, by analyzing the temporal decay of the field amplitude using a filter-diagonalization method on a Fourier basis [17], we are able to obtain two distinct resonance frequencies and their linewidths. Using this information, we compare the theoretical transmission spectrum with FDTD results shown in Fig. 5(b) and obtain excellent agreement between the two. (In using (28), $t_d = 1$ and $r_d = 0$, since the direct transmission, i.e., the transmission coefficient for the wave inside the waveguide in the absence of the cavities, is 100%.)

The theory can also be applied to general cases where the matrix C is not an identity matrix, in which case Fano interference occurs. As an example, we consider the transmission spectrum for light normally incident upon a single slab photonic crystal slab structure, as shown in Fig. 6(a). The slab is constructed by introducing a periodic array of air holes into a high-index guiding layer [18]. The dielectric constant is chosen to be 12, which approximates to that of silicon at optical frequencies. The radius of air holes is $0.2a$, where a is the lattice constant, and the thickness of the slab is a. For this structure, a modal analysis reveals the existence of two modes with frequencies in close proximity to each other, as shown in Fig. 6(b). Both modes possess odd symmetry with respect to the mirror plane at the center of the slab. The transmission through the system is shown in Fig. 6(c). The open circled spectrum is the FDTD result and the solid line is the spectrum predicted by analytic theory. To determine the parameters for the theory plot, we obtain the resonance frequency and the width by Fourier transform of the temporal decaying tail of the resonances, and determine t_d with the model of a uniform dielectric slab with an effective dielectric function [18]. We again see excellent agreement between the theory and the FDTD results. Thus, the FDTD results completely validate our coupled mode theory analysis.

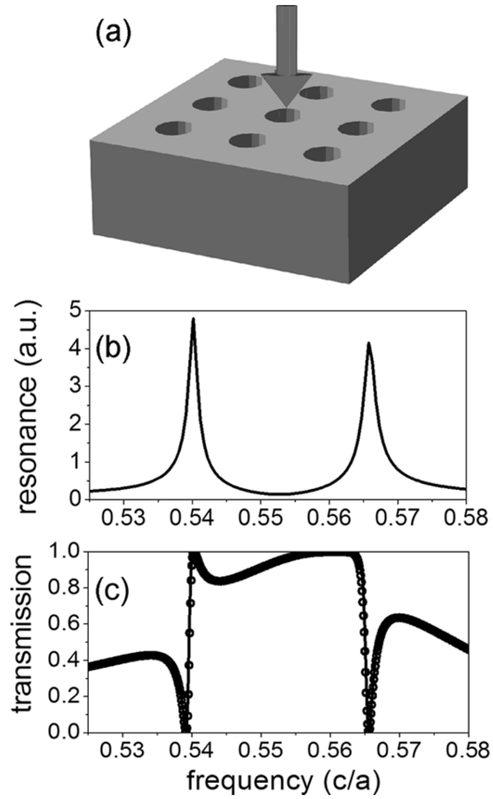

Fig. 6. (a) Schematic of a photonic crystal slab structure. The arrow represents the direction of incident light. The structure has thickness of $1a$, and dielectric constant of 12. Within the slab, there are air holes of radius $0.2a$. (b) Resonance amplitude of two modes in the structure that are excited by normally uincident light. The two modes both have odd symmetry with respect to the mirror plane parallel to the slab. (c) Transmission spectrum upon normally incident light. Solid line is the analytic theory and the open circles are FDTD simulations.

V. SUMMARY

We introduced a general temporal coupled-mode theory for optical resonators. Using this theory, we prove a general criterion for the existence of nonorthogonal modes in passive optical resonator systems. We note that this theory can be extended to include both radiation loss and material loss in a phenomenologically standard way [7], by introducing additional decay in the diagonal elements of the Γ matrix. The Γ matrix now consists of two parts: $\Gamma_{\rm ports}$, which describe the decay of resonance due to coupling to the ports, and $\Gamma_{\rm loss}$, which represents coupling to a continuum of radiation modes. The result in (4) is now expressed in $\Gamma_{\rm ports}$ only, and thus the existence of nonorthogonal modes is unaffected. We expect such theory to be important for any optical devices that employ multimode resonator systems, including applications such as optical sensors and switches.

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