

# Temporal coupled-mode theory for the Fano resonance in optical resonators

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We present a theory of the Fano resonance for optical resonators, based on a temporal coupled-mode formalism. This theory is applicable to the general scheme of a single optical resonance coupled with multiple input and output ports. We show that the coupling constants in such a theory are strongly constrained by energy-conservation and time-reversal symmetry considerations. In particular, for a two-port symmetric structure, Fano-resonant line shape can be derived by using only these symmetry considerations. We validate the analysis by comparing the theoretical predictions with three-dimensional finite-difference time-domain simulations of guided resonance in photonic crystal slabs. Such a theory may prove to be useful for response-function synthesis in filter and sensor applications. © 2003 Optical Society of America

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## 1. INTRODUCTION

The Fano resonance line shape appears in the optical transmission and reflection spectra for a wide variety of structures, such as metallic or dielectric gratings<sup>1–13</sup> and side-coupled waveguide-cavity systems.<sup>14</sup> The resonance occurs from interference between a direct and a resonance-assisted indirect pathway and typically exhibits a sharp asymmetric line shape with the transmission coefficients varying from 0 to 100% over a very narrow frequency range. Recently, Fano effects have been exploited in narrowband optical filters, polarization selectors, modulators, switches; sensors<sup>5–7,10,13</sup> and have also been observed in photonic crystal slab structures.<sup>15,16</sup>

The theory of Fano resonance is very well developed in metallic and dielectric grating structures. In early studies, the Fano resonance phenomenon in these structures was attributed to the presence of leaky modes supported by the gratings.<sup>2,3</sup> Later, extensive theoretical and numerical studies were devoted to the study of the spatial coupling of such leaky modes to the external waves.<sup>5–9,11,12</sup> However, given the ubiquitous nature of Fano effects, which are not restricted to the grating structures, it is clearly of interest to construct a theory that illustrates the fundamental aspects of the interference behavior.

In this paper we develop a general theory of transport processes from multiple input and output ports through a single-mode optical resonator. The theory incorporates the effects of both direct and indirect pathways and is thus applicable to any single-mode resonator structure that exhibits the Fano effect, including all the examples cited above. We show that the coupling constants in this theory are strongly constrained by energy-conservation and time-reversal symmetry considerations. In particu-

lar, in a two-port system with mirror symmetry, the coupling constants are in fact completely constrained, and the Fano line shape becomes a natural consequence. We believe that our theory, being formulated in a general fashion, should therefore prove to be useful for response-function synthesis in filter and sensor applications.

## 2. THEORY

We develop our theory on the basis of the coupling of modes in a time-dependent formalism for optical resonators.<sup>17</sup> The theoretical model, schematically shown in Fig. 1, consists of a single-mode optical resonator coupled with  $m$  ports, labeled 1, 2, ...,  $m$ . The dynamic equations for the amplitude  $a$  of the resonance mode can be written as

$$\frac{da}{dt} = \left( j\omega_0 - \frac{1}{\tau} \right) a + (\langle \kappa |^* ) |s_+\rangle, \quad (1)$$

$$|s_-\rangle = C |s_+\rangle + a |d\rangle, \quad (2)$$

where  $\omega_0$  and  $\tau$  are the center frequency and the lifetime of the resonance, respectively. The amplitude  $a$  is normalized such that  $|a|^2$  corresponds to the energy inside the resonator.<sup>17</sup> The resonant mode is excited by the incoming waves

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

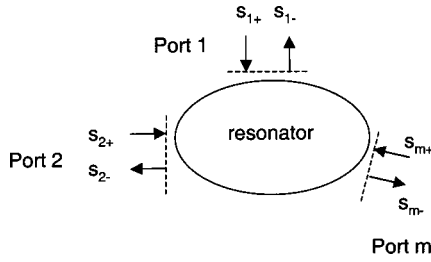


Fig. 1. Schematic of an optical resonator system coupled with multiple ports. The arrows indicate the incoming and outgoing waves. The dashed lines are reference planes for the wave amplitudes in the ports.

from ports 1 to  $m$ , respectively, with the coupling constants

$$\langle \kappa |^* = \begin{pmatrix} \kappa_1 \\ \kappa_2 \\ \vdots \\ \kappa_m \end{pmatrix}.$$

(For compactness of presentation we adopt Dirac's bracket notation to describe vectors that are indexed to the labels of the ports.) The resonant mode, once excited, couples with the outgoing waves

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

at the ports with the coupling constants

$$|d \rangle = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_m \end{pmatrix}.$$

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 a scattering matrix  $C$ . The presence of the direct pathway is an essential aspect of the Fano effect. Hence the matrix  $C$  here must be taken to be an arbitrary scattering matrix, i.e., any unitary and symmetric matrix.

Equations (1) and (2) represent a generalization of the standard temporal coupled-mode theory,<sup>17</sup> in which  $C$  is a diagonal matrix. Our theory thus assumes the same regime of validity as the standard temporal-coupled-mode theory; i.e., this approach is strictly valid only when the width of the resonance is far smaller than the resonance frequency. It has been shown in Ref. 17 that in this regime the coupling constants can be taken to be frequency independent and that the frequency shift due to the expo-

ponential decay of the mode to the ports is a second-order effect and can be incorporated into the theory through a renormalization of  $\omega_0$ .

The coefficients  $\kappa$ ,  $d$ , and  $C$  are not independent; rather, they are related by energy-conservation and time-reversal symmetry constraints. Below we will exploit the consequence of these constraints to develop a minimum set of parameters that completely characterize the system. First, for externally incident excitations  $|s_+ \rangle$  at a frequency  $\omega$ , we can write the scattering matrix  $S$  for the system described by Eqs. (1) and (2) as

$$|s_- \rangle = S|s_+ \rangle = \left[ C + \frac{|d \rangle \langle \kappa|^*}{j(\omega - \omega_0) + 1/\tau} \right] |s_+ \rangle. \quad (3)$$

Since the scattering matrix has to be symmetric because of time-reversal symmetry, we have

$$|d \rangle \langle \kappa|^* = |\kappa \rangle \langle d|^*. \quad (4)$$

(Thus the coefficients  $|\kappa \rangle$  and  $|d \rangle$  are not independent and must satisfy  $d_1 \kappa_2 = d_2 \kappa_1$ , etc). Also, with incoming-wave amplitudes  $|s_+ \rangle$ , the amplitude of the resonant mode is

$$a = \frac{\langle \kappa |^* |s_+ \rangle}{j(\omega - \omega_0) + 1/\tau}. \quad (5)$$

Instead of considering the case in which the resonator is excited by externally incident waves  $|s_+ \rangle$ , let us now consider an alternative situation in which the external incident wave is absent, i.e.,  $|s_+ \rangle = 0$ , and at  $t = 0$  there is a finite amplitude of the resonance. At  $t > 0$ , the resonant mode decays exponentially into the two ports, as

$$\frac{d|a|^2}{dt} = -\left(\frac{2}{\tau}\right)|a|^2 = -\langle s_- | s_- \rangle = -|a|^2 \langle d | d \rangle, \quad (6)$$

which requires that

$$\langle d | d \rangle = 2/\tau. \quad (7)$$

Now, let us perform a time-reversal transformation for the exponential decay process as described by Eq. (6). The time-reversed case is represented by feeding the resonator with exponentially growing waves at a complex frequency  $\omega = \omega_0 - j(1/\tau)$ , with amplitudes at  $t = 0$  equal to  $|s_- \rangle^*$ . Such excitations cause a resonance amplitude  $a^*$  at  $t = 0$  to grow exponentially in time.<sup>17</sup> Using Eq. (5) at the complex frequency  $\omega = \omega_0 - j(1/\tau)$ , we have

$$a^* = \frac{\langle \kappa | s_- \rangle^*}{2/\tau} = \frac{\langle \kappa | d \rangle a^*}{2/\tau},$$

and therefore

$$\langle \kappa | d \rangle = 2/\tau = \langle \kappa | d \rangle^*. \quad (8)$$

Combining Eqs. (4), (7), and (8), we are led to an important conclusion:

$$|\kappa \rangle = |d \rangle. \quad (9)$$

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

$$0 = C|s_- \rangle^* + a^*|d \rangle = a^*C|d \rangle^* + a^*|d \rangle, \quad (10)$$

Thus the coupling constants  $|d\rangle$  have to satisfy a further condition:

$$C|d\rangle^* = -|d\rangle. \quad (11)$$

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

To check that Eqs. (9) and (11) indeed produce a self-consistent temporal coupled-mode theory, we need to ensure that the scattering matrix  $S$ , as defined by Eq. (3), is unitary. For this purpose, we note that

$$\begin{aligned} SS^+ &= CC^+ + \frac{(2/\tau)|d\rangle\langle d|}{(\omega - \omega_0)^2 + (1/\tau)^2} \\ &+ \frac{C|d\rangle^*\langle d|}{-j(\omega - \omega_0) + (1/\tau)} + \frac{|d\rangle\langle d|^*C^+}{j(\omega - \omega_0) + (1/\tau)}. \end{aligned} \quad (12)$$

Taking advantage of Eq. (11) and its complex conjugate,

$$\langle d|^*C^+ = (\langle d|C^T)^* = (C|d\rangle^*)^+ = -(|d\rangle)^+ = -\langle d|, \quad (13)$$

we can indeed prove the unitary property of the matrix  $S$ :

$$\begin{aligned} SS^+ &= CC^+ + \frac{(2/\tau)|d\rangle\langle d|}{(\omega - \omega_0)^2 + \tau^2} + \frac{-|d\rangle\langle d|}{-j(\omega - \omega_0) + (1/\tau)} \\ &+ \frac{-|d\rangle\langle d|}{j(\omega - \omega_0) + (1/\tau)} = CC^+ = I. \end{aligned} \quad (14)$$

Equations (1)–(14) are applicable to the general problem of a single optical mode coupled with multiple input and output ports. Below, we will apply the general formalism to two-port structures. In this case, it can be shown that once the magnitudes of the coupling constants  $d_1$  and  $d_2$  are fixed, the phases of the coupling constants can be determined from the scattering matrix  $C$  of the direct process. The theory can be further simplified, however, when we consider structures with mirror symmetry. For these structures, if we place the reference planes symmetrically on each side of the structure with respect to the mirror plane, the scattering matrix has to be such that the two diagonal elements are equal. Thus we have  $d_1^2 = d_2^2$ . The scattering matrix for the direct transport process also acquires a special form<sup>17</sup>:

$$C = \exp(j\phi) \begin{bmatrix} r & jt \\ jt & r \end{bmatrix}, \quad (15)$$

where  $r$ ,  $t$ , and  $\phi$  are real constants with  $r^2 + t^2 = 1$ . Using Eqs. (7) and (11), we can determine  $d_1$  and  $d_2$ , and consequently the scattering matrix  $S$  for the overall system as

$$\begin{aligned} S &= \exp(j\phi) \left\{ \begin{bmatrix} r & jt \\ jt & r \end{bmatrix} \right. \\ &+ \frac{1/\tau}{j(\omega - \omega_0) + 1/\tau} \begin{bmatrix} -(r \pm jt) & \mp(r \pm jt) \\ \mp(r \pm jt) & -(r \pm jt) \end{bmatrix} \Bigg\}. \end{aligned} \quad (16)$$

Here the  $\pm$  sign corresponds to the case where the resonant mode is even (odd) with respect to the mirror plane,

in which case  $d_1 = +(-)d_2$ . From Eq. (16), the intensity reflection coefficient  $R$  is therefore

$$R = \frac{r^2(\omega - \omega_0)^2 + t^2(1/\tau)^2 \mp 2rt(\omega - \omega_0)(1/\tau)}{(\omega - \omega_0)^2 + (1/\tau)^2}. \quad (17)$$

A symmetric Lorentzian line shape is reproduced only when either  $r$  or  $t$  is zero. In all other cases, the system exhibits a Fano asymmetric line shape. Thus our theory directly predicts the line-shape function of the Fano phenomena.

### 3. NUMERICAL VALIDATION OF THE THEORY

The theoretical derivation above should be applicable to any single-mode optical resonator system. To check the validity of the theory, we compare the theoretical predictions to first-principles simulations of one type of optical resonance: the guided resonance in a photonic crystal slab. For definiteness, we consider a crystal consisting of a square lattice of air holes, each with a radius of  $0.2a$ , where  $a$  is the lattice constant, introduced into a dielectric slab with a dielectric constant of 12 and a thickness of  $0.55a$ . We find that the two lowest-frequency resonant states at  $\Gamma$  occur at  $0.37$  and  $0.39(c/a)$ , where  $c$  is the speed of light in vacuum.

We shall now focus on these resonances and investigate their line shapes. Using finite-difference time-domain simulations, we calculate the transmission spectra of light that is normally incident on the slab [Fig. 2(a)].

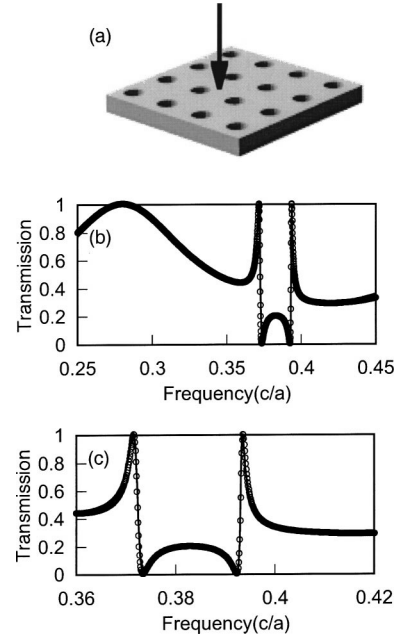


Fig. 2. (a) Photonic crystal structure consisting of a square lattice of air holes of radius  $0.2a$  in a dielectric slab with dielectric constant 12 and a thickness of  $0.55a$ . The arrow indicates the direction of the incident light. (b) The intensity transmission spectrum through such a structure. The circles are the results from the finite-difference time-domain simulations. The solid curve is determined from analytic theory as represented by Eq. (16). (c) The same plot as in (b), except that the frequency range is now restricted to  $[0.36(c/a), 0.42(c/a)]$  to exhibit further details of the resonance line shape.

The simulated transmission spectrum, shown as circles in Fig. 2(b), consists of Fano resonant line shapes superimposed on a smooth Fabry–Perot background.<sup>18</sup> To compare the simulations with theory, we determine from the simulations the frequency and the width of the resonance by studying the exponential temporal decay of the resonance amplitude after the excitation. The scattering matrix  $C$  for the direct transmission process is established by fitting the background in the simulated spectrum to the transmission coefficients through a uniform slab with the same thickness and with an effective dielectric constant. Using these parameters, we then calculate the theoretical spectrum using Eq. (16) and plot it as a solid curve in Fig. 2(b) and 2(c). There is excellent agreement between theory and simulations.

#### 4. FINAL REMARKS

In concluding, we note that for structures in which the resonances are sufficiently close to each other, a general theory incorporating multiple resonances is needed. Such a theory will be developed in future research. In addition, while the scattering-matrix approach has been used in the analysis of gratings<sup>4</sup> and in the general case of arbitrary scatters,<sup>19</sup> and many aspects of the Fano resonance can be obtained in a structure-independent fashion by using the symmetry properties of the scattering matrix alone (as previously reported in studies of phase-coherent transport in mesoscopic semiconductors),<sup>20</sup> our theory does contain additional dynamic information about the resonance amplitude. With this information, temporal coupled-mode theory can be readily applied in situations with more than one resonant mode and with nonlinearity<sup>17</sup>—situations in which a straightforward application of scattering-matrix formalism alone would have been more difficult. Thus we believe that the theory presented here should be useful for synthesizing response functions in filter and sensor applications.

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