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Reconstructing the scattering matrix of photonic systems from quasinormal modes

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ABSTRACT
The scattering matrix is a fundamental tool to quantitatively describe the properties of resonant systems. In particular, it enables the understanding of many photonic devices of current interest, such as photonic metasurfaces and nanostructured optical scatterers. In this contribution, we show that the scattering matrix of a photonic system is completely determined by its quasinormal modes, i.e., the self-sustaining electromagnetic excitations at a complex frequency. On the basis of temporal coupled-mode theory, we derive an expression for the expansion of the scattering matrix on quasinormal modes, which is directly applicable to an arbitrary number of modes and input/output channels. Our theory does not require any *ad-hoc* assumptions, such as the fitting of an additonal nonresonant background.
We validate and discuss the theoretical formalism with some illustrative examples. This demonstrates that the theory represents a powerful and predictive tool for calculating the highly structured spectra of resonant nanophotonic systems, and, at the same time, a key for unravelling the physical mechanisms at the heart of such intricate spectral structures.
Keywords: scattering matrix, quasinormal modes, resonant states, theoretical photonics, photonic crystals.

1. INTRODUCTION

The scattering matrix constitutes an important tool in multiple fields of science, such as nuclear physics, electronic transport, or classical electrodynamics [1,2]. In particular, it plays an essential role in helping us to understand intriguing optical phenomena, such as Fano resonances in optical systems [3] or scattering dark states [4], and to tailor the properties of novel photonic devices, like photonic metasurfaces [5] or hybrid plasmonic-photonic nanoresonators [6].

These electromagnetic systems typically display a highly structured spectral response, with multiple resonances in the spectrum. The resonances are associated with *quasinormal modes* (also called *resonant states*), i.e., complex-frequency solutions of Maxwell's equations with outgoing-wave boundary conditions [7-9]. In order to decipher, understand, and engineer the behaviour of complex optical systems, it is vital to unravel the connection between the scattering matrix and the underlying quasinormal modes.

In this contribution, we develop a rigorous and general theory for the expansion of the scattering matrix of electromagnetic systems on quasinormal modes. The method is based on the framework of temporal coupled-mode theory for optical resonators [3,10]. Such framework has been effectively used to study the transmission of gratings and photonic-crystal structures [3,10-12] and the scattering cross section of nanoparticles [4]. However, in these applications, coupled-mode theory has been usually restricted to only one or two modes of the optical system, with the residual spectral response being taken into account with a slowly varying frequency-dependent background, fitted from independent simulation data [3,10,11]. Our theory provides a direct and general relation between the coefficients of the scattering-matrix expansion and the values of the complex modal field at the input-output ports of the system. Therefore, the theory is directly applicable to any number of multiple overlapping modes, without any restriction on the width or decay rate, and to an arbitrary configuration of input-output channels. These characteristics make it especially suitable for a first-principle description of complex photonic systems. Notably, since the formalism is based on general coupled-mode theory, its range of applicability goes beyond that of classical electrodynamics.

2. THEORY

The starting point for our theory is the formalism of temporal coupled-mode equations [3,10]. We assume that the incoming electromagnetic field of an optical system is expanded on a set of m input ports: $\boldsymbol{E}_{in} = \sum_\alpha s_{+\alpha} \boldsymbol{E}_\alpha^{(+)}$. The incoming field is dynamically coupled to a number n of quasinormal modes. In vector notation, this fact can be expressed in terms of the $m\times n$ coupling matrix D:

$$\frac{d}{dt}\boldsymbol{a} = i\,(\Omega + i\,\Gamma)\boldsymbol{a} + D^T \boldsymbol{s}_+, \tag{1}$$

where the vectors $\boldsymbol{a}$ and $\boldsymbol{s}_+$ contain the coefficients of the expansion of the field in terms of quasinormal modes and input channels, respectively.

The outgoing field is similarly expanded on a basis of output ports, $\boldsymbol{E}_{out} = \sum_\alpha s_{-\alpha}\boldsymbol{E}_\alpha^{(-)}$. The amplitude of each outgoing wave is the result of two different contributions: a direct channel (accounted for by a $m\times m$ matrix C) and a resonance mediated channel:

$$\boldsymbol{s}_- = C\,\boldsymbol{s}_+ + D\,\boldsymbol{a}. \tag{2}$$

Using the same notation, quasinormal modes are the solutions of the eigenproblem for the non-Hermitian Maxwell operator $H = \Omega + i\Gamma$ (Ω and Γ being Hermitian operators) with the complex eigenfrequencies $\tilde{\omega}_j$:

$$(\Omega + i\,\Gamma)\,\tilde{\boldsymbol{a}}_j = \tilde{\omega}_j\,\tilde{\boldsymbol{a}}_j. \tag{3}$$

We also define the *scattering eigenvectors* $\boldsymbol{b}_j = D\,\tilde{\boldsymbol{a}}_j$, i.e., the expansion coefficients of the modal field of the quasinormal modes on the output ports of the system. In practice, quasinormal modes can be computed by numerically solving the eigenproblem for Maxwell equations with outgoing boundary conditions. The scattering eigenvectors depend only on the far-field behaviour of the resonant states, and, for this reason, they can be obtained without computing the full spatial distribution of the electromagnetic field of the corresponding quasinormal modes.

The scattering matrix of the system connects the coefficients of the outgoing field with the coefficients of the incoming field and, in the frequency domain (assuming the frequency dependence $e^{i\omega t}$), it can be written as:

$$S = C - iD\,(\omega - \Omega - i\Gamma)^{-1}\,D^T. \tag{4}$$

Using the biorthogonal properties of quasinormal modes [13], the scattering matrix can be recast in the form

$$S = C + i\sum_j \frac{\lambda_j}{\omega - \tilde{\omega}_j}\boldsymbol{b}_j\boldsymbol{b}_j^T. \tag{5}$$

In the following, we will briefly discuss how to derive the values of the expansion coefficients λ_j. In order to do so, we have to recall some additional relations among the quantities in Eqs. (1) and (2), which were originally demonstrated in Refs. [3] and [10] on the basis of electromagnetic reciprocity and time-reversal symmetry considerations:

$$\Gamma = \tfrac{1}{2}D^\dagger D \qquad \text{and} \qquad CD^* = -D. \tag{6}$$

It can be shown that these equations imply the additional relation

$$\sum_i C\,\boldsymbol{b}_i^*\,Q_{ij}^{*\,-1} - \lambda_j\boldsymbol{b}_j = 0\,, \tag{7}$$

with the matrix Q defined as: $Q_{ij} = i\,\boldsymbol{b}_i^\dagger\boldsymbol{b}_j/(\tilde{\omega}_j - \tilde{\omega}_i^*)$. Equation (7) can be solved in a least-square sense as a function of λ_j. The solution, then, allows us to obtain the values of the coefficients in Eq. (5) and to carry out the quasinormal expansion of the scattering matrix. The least-square solution of Eq. (7) is

$$\lambda_j = \frac{\sum_{ik} Q_{ij}^{-1} Q_{kj}^{*\,-1}\boldsymbol{b}_i^T C^\dagger C\,\boldsymbol{b}_k^*}{\sum_i Q_{ij}^{-1}\,\boldsymbol{b}_i^T C^\dagger \boldsymbol{b}_j}. \tag{8}$$

This last equation, together with Eq. (5), represents the main result of the present contribution. The quasinormal-mode expansion of the scattering matrix that we derive in Eq. (5) is similar to the Breit-Wigner formula of nuclear physics [2]. However, there is a fundamental difference in the expression of the expansion coefficients (Eq. 7): the coefficient of each resonant term in the expansion depends on the frequencies and the amplitudes of all the other modes via the specifically introduced coupling matrix Q. This matrix accounts for the effective interaction among different quasinormal modes that originates from the coupling to a common external environment. This characteristic reflects in the fact that, whereas the Breit-Wigner formula is restricted to the case of non-overlapping resonances, no such limitation applies to the present theory. Thus, the theory can be used in a straightforward way to model systems characterized by an arbitrary number of closely spaced resonant states.

3. APPLICATIONS

As an illustrative example of the application of the theory, we consider a simple Fabry-Perot resonator made of a dielectric slab in air. The refractive index of the dielectric is n_d. Since the structure is translationally invariant in a two-dimensional plane, we limit ourselves to the subspace of electromagnetic solutions with a fixed in-plane wavevector k, and we assume $k = 0$. The complex eigenfrequencies of the quasinormal modes of the structure can be worked out analytically and they have the form

$$n_d\frac{\tilde{\omega}_j}{c}L = j\pi - i\ln(r), \qquad j = 0, \pm1, \pm2, \ldots \tag{9}$$

where $r = (n_d - 1)/(n_d + 1)$ is the reflection coefficient of the air-dielectric interface. The two input-output ports correspond to plane waves propagating in the upper and lower region with respect to the slab, respectively. The expressions of the scattering eigenvectors can be obtained directly from symmetry considerations, since all quasinormal modes are even or odd with respect to the inversion along the axis perpendicular to the slab. It can be demonstrated that the expression in Eqs. (5) and (8) for the scattering matrix expansion does not depend on the global normalization constant of the scattering eigenvectors. Therefore, we are free to choose the normalization constant and we define the scattering eigenvectors

$$\boldsymbol{b}_j = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad j \text{ even}; \qquad \boldsymbol{b}_j = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad j \text{ odd}. \tag{10}$$

Finally, assuming that the set of quasinormal modes is complete, we take the 2×2 identity matrix as the direct coupling matrix, i.e., $C = I_{2\times 2}$.

Putting together all these ingredients, we can compute the scattering matrix of the system by applying Eq. (5) with the coefficients of Eq. (8). The resulting scattering matrix allows us to obtain all the scattering quantities of the system, such as the transmission and reflection intensities. As an example, the transmission spectrum obtained from the quasinormal-mode expansion is plotted in Fig. 1 and compared with the exact analytical result. The agreement between the curves is excellent, and it improves with the increasing of the cut-off for the set of quasinormal modes employed in the expansion. Notably, these results clearly prove that it is possible to derive the scattering properties on the entire frequency range only from the knowledge of the quasinormal modes of the system.

The validity of the quasinormal-mode expansion of the scattering matrix can be further demonstrated in the case of more complex systems. For instance, in Fig. 2 we show the transmission spectrum of a two-dimensional period structure of L-shaped air-holes patterned in a high-index dielectric slab. The frequencies and eigenvectors of the quasinormal modes have been numerically computed with the finite-element method [14]. Even in this case, we assume the identity as the direct coupling matrix *C*. The result obtained from the quasinormal-mode expansion of the scattering matrix is compared with an independent calculation by the Fourier modal method [15]. The agreement between the curves is very good, confirming the validity of the quasinormal-mode expansion of the scattering matrix. Moreover, the comparison demonstrates that the first-principle description provided by the theory is complete and accurate, without the need for fitting any *ad-hoc* background response for the direct coupling channel.

4. CONCLUSIONS

In this contribution, we have illustrated a method to expand the scattering matrix of optical systems on the basis of quasinormal modes and we have validated it with benchmark examples. The theory can be applied in a straightforward way to systems with an arbitrary number of resonant modes and input-output channels. Moreover, it only requires the knowledge of the complex eigenfrequencies and the far-field profiles of the quasinormal modes of the system, eliminating the need for introducing a frequency-dependent background channel. All these characteristics make the theory a powerful first-principle tool for understanding and tailoring the optical properties of complex photonic systems.

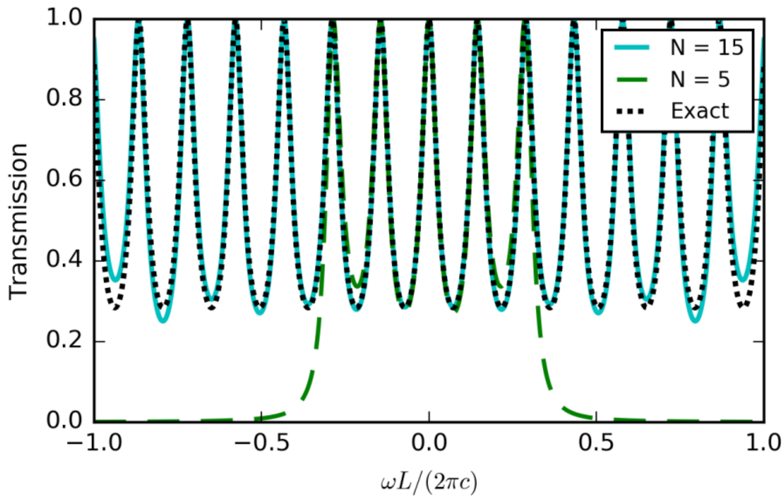

Figure 1: normal-incidence transmission spectrum of a Fabry-Perot resonator made of a dielectric slab with refractive index n_d = 3.46 in air. Solid and dashed curves: data computed from the quasinormal-mode expansion of the scattering matrix with N = 15 and N = 5 modes, respectively. Dotted curve: exact analytical result.

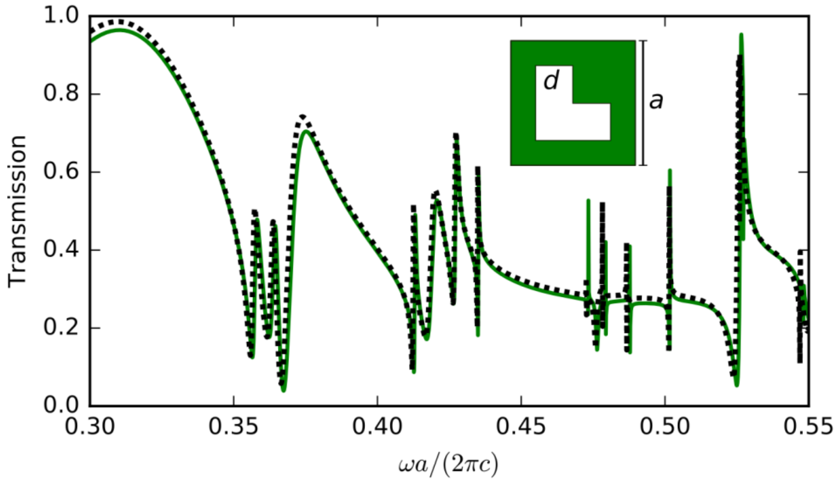

Figure 2: normal-incidence transmission spectrum of a two-dimensional periodic array (a = lattice constant) of L-shaped air holes. The structures are partially etched (at half depth) in a dielectric slab (ε = 12.1) of thickness t = 0.5a. The inset shows a top view of the unit cell (d = 0.3a). The results from the quasinormal-mode expansion of the scattering matrix (solid line) are compared with full-wave simulation data (dotted line).

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