# A Coupled-Mode Theory Approach for Consolidating Nonlinearities with Quasinormal Modes

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**Abstract:** A rigorous nonlinear framework for modeling resonant cavities is presented, reconciling perturbation theory/coupled-mode theory approach with quasinormal modes. The framework is tested in characteristic guided and free-space resonant cavities. © 2021 The Author(s)

#### 1. Introduction

Nanophotonic resonant cavities constitute a key element in integrated photonic/plasmonic and quantum systems. Due to their ability to confine light both spatially and temporally, optical cavities enable elaborate functionalities and are particularly important for low-power nonlinear interactions, lasing applications, and switching/routing. For the analysis/design of optical cavities, rigorous theoretical/computational frameworks have been developed (see, e.g., Ref. [1] and the references therein), which allow for efficiently assessing their response as well as gaining physical insight. Nevertheless, as the trend for contemporary devices is to further shrink their size leading to increased light leakage, classical frameworks fail to capture the inherently leaky nature of the involved cavities. As a result, a new approach has been recently established, based on quasinormal modes (QNMs) [2], i.e., non-orthogonal modes that are the eigenvectors of the source-free Maxwell's equations in non-Hermitian systems.

Continuously over the past few years, QNM theory is being significantly developed and gradually introduced in established mathematical formulations for efficient resonator description, such as the temporal coupled-mode theory (CMT) framework [3, 4]. However, thus far the approaches are limited to linear resonators [3, 4] or are focused solely on free-space nanocavities [2, 5]. It is our prime goal here to present a unified nonlinear CMT framework (additionally using perturbation theory to include nonlinear phenomena) which incorporates the leaky nature of QNMs and is appropriate for handling either guided-wave or free-space cavities involving contemporary bulk and sheet materials, such a as graphene.

## 2. Nonlinear Framework Attributes

The proposed framework is based on correctly taking into account the leaky nature of QNMs which exponentially diverge away from a cavity with non-negligible radiation losses. This is rigorously done by resorting to the unconjugated Lorentz reciprocity theorem that holds regardless of the lossy nature of the involved materials (e.g. for plasmonic or graphene-based cavities) and by moreover terminating the computational domain with perfectly matched layers (PMLs). Ultimately, the effects of the nonlinearities in the system are described by a single (complex-valued) quantity  $\Delta \widetilde{\omega}$ , encapsulating both resonance frequency shifts and linewidth deformations [5, 6]

$$\frac{\Delta \widetilde{\omega}}{\widetilde{\omega}_{0}} = -\frac{\iiint_{V} \mathbf{P}_{\text{pert}} \cdot \mathbf{E}_{0} dV}{\iiint_{V+V_{\text{PML}}} \varepsilon_{0} [\partial \{\omega \varepsilon_{r}(\omega)\} / \partial \omega] \mathbf{E}_{0} \cdot \mathbf{E}_{0} dV - \iiint_{V+V_{\text{PML}}} \mu_{0} \mathbf{H}_{0} \cdot \mathbf{H}_{0} dV}.$$
(1)

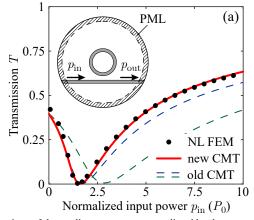
The use of the unconjugated Lorentz reciprocity theorem is reflected in the denominator of Eq. (1) which is not proportional to the stored energy in the system but is rather a complex-valued quantity. Moreover, the contribution of the PMLs suppresses the spatial divergence of the QNMs without affecting their properties, resulting in a constant  $\Delta \tilde{\omega}$  regardless of the computational window dimensions [2, 6]; this is not true for the classical, conjugated approach [1].

When nonlinear perturbations are considered, for the introduction of Eq. (1) in the CMT formalism  $\Delta \widetilde{\omega}$  should be expressed as a function of the stored energy in the cavity; this is straightforward for normal modes with a well-defined stored energy, but not readily achievable for a leaky QNM. Still, using the definition of the resistive quality factor as  $Q_{\rm res} = {\rm Re}\{\widetilde{\omega}_0\}W_{\rm stor}/P_{\rm res}$  one can implicitly introduce the stored energy in the formulation so that now  $\Delta\widetilde{\omega} = \Delta\widetilde{\omega}(W_{\rm stor})$  [6], an approach that is necessary for the nonlinear CMT framework development. Importantly, only the well-behaved  $P_{\rm res}$  has to be calculated using the diverging eigenvector, which is straightforward since the integration

is limited inside the cavity itself; expressions involving  $W_{\text{stor}}$  are translated into CMT-based quantities (i.e., proportional to the cavity mode amplitude since  $W_{\text{stor}} \equiv |a|^2$ ) and are calculated through simple polynomial or time-dependent ordinary differential equations and not by the spatially diverging mode. It is noted that the proposed transformation is not restricted to the type of the nonlinearity but is very general and can by applied for an arbitrary nonlinear bulk susceptibility  $\chi^{(n)}$  and/or surface conductivity  $\sigma^{(n)}$  when graphene or other 2D materials are concerned.

## 3. Nonlinear Framework Applications

To demonstrate the capabilities of the developed framework, a guided-wave system consisting of a side-coupled slab ring resonator is firstly examined [inset of Fig. 1(a)]. The parameters of the system are chosen to reproduce a highly leaky behavior, with a radiation quality factor of only 140. As revealed from Fig. 1(a), the unconjugated framework can accurately predict the nonlinear response of the cavity (verified by full-wave nonlinear finite-element simulations in the CW case), in sharp contrast to the traditional, conjugated one.



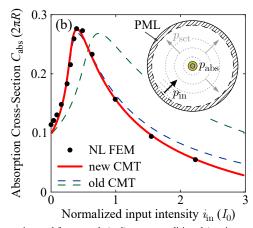


Fig. 1. Comparison of the nonlinear response as predicted by the proposed, unconjugated framework (red) versus traditional (conjugated) CMT with (blue) or without (green) applying the indirect energy definition through  $Q_{\rm res}$ . The horizontal axis is normalized with respect to an input power/intensity level characteristic of the nonlinearity. (a) Transmission of a side-coupled, slab ring resonator ( $\varepsilon_r = 6 - j0.0022$ ,  $R = 0.79~\mu m$ ) at 1550 nm. (b) Absorption cross-section of a plasmonic core-shell nanorod ( $\varepsilon_m = -34 - j0.4$ ,  $\varepsilon_d = 2.1$ , R = 152 nm) at 814 nm.

The framework was also tested in the case of a highly dispersive free-space plasmonic core-shell nanorod with a nonlinear dielectric core, operating in the infrared [inset of Fig. 1(b)]. Despite the ultra-low radiation quality factor of the plasmonic system  $[Q_{rad} = 40]$ , the unconjugated framework still retrieves correctly the absorption cross-section of the nanoparticle, as the input power raises. Based on the presented capabilities, the proposed framework constitutes a significant contribution to the fast and accurate analysis and design of contemporary nonlinear nanocavities.

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