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A multimode quasi-normal mode framework for nonlinear harmonic generation with 2D materials

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Abstract: In this work, we present a multimode framework for linear and nonlinear modal calculations in non-Hermitian systems comprising 2D materials. The framework is based on the ability to appropriately expand both the linear and nonlinear responses of a resonant cavity in terms of the supported quasi-normal modes. Through numerical simulations, we find that the proposed framework is efficient and extremely accurate, even when complex contemporary photonic systems incorporating 2D materials are involved.

Non-Hermitian cavities, i.e., resonant systems with radiation leakage and resistive loss, support quasi-normal modes (QNMs), whose properties are not as well-defined as those of normal modes supported by Hermitian systems. QNMs exhibit interesting but cumbersome properties, with the most notable being the unphysical spatial exponential divergence of the field components outside the resonant cavity, complicating the process of their normalization. Lately, the study of QNMs has produced very interesting results by providing the appropriate normalization needed to regularize this mode divergence [1-2]. In effect, this important fact led to the development of elegant techniques to reconstruct the full linear spectrum of a system using the QNMs it supports [3]. However, the study of expansions that additionally include nonlinear interactions received much less attention [4-5]. Additionally, although the methods presented thus far cover a wide range of material configurations (dielectric and plasmonic scatterers and metasurfaces, photonic crystals, etc.), none has focused on the contemporary family of 2D materials (e.g., graphene, transition metal dichalcogenides, black phosphorus, etc.) which, among others, possess unique nonlinear properties. In this work, we present such a complete methodology, beginning from the careful introduction of 2D materials in the linear QNMs framework through their natural representation as infinitesimally thin layers and subsequently progressing to additionally include their nonlinear properties through the demonstration of the third harmonic generation effect [5]. We also rigorously take into account material dispersion by expanding the established finite-element method using appropriate surface auxiliary fields [3,5]. Thus, we successfully provide with the proper normalization that correctly captures the full complexity of 2D materials including infinitesimal thickness, dispersion, loss, and anisotropy, applicable either in linear or nonlinear systems.

The developed nonlinear multimode framework is validated through two indicative resonant structures comprising graphene [Fig. 1(a)], i.e., the most prominent 2D material. Graphene supports tightly confined surface plasmons in the THz regime, whose tight confinement further enhances its inherent strong nonlinear response. The first example that is examined consists of a single graphene strip lying on a glass substrate. The second is a metasurface made of periodically arranged graphene strips on a metal-backed substrate to operate in reflection. The response (both linear and nonlinear) of the two systems is studied using the developed QNMs framework and validated through (nonlinear) full-wave simulations. The results of Fig. 1(b-e) show that excellent agreement is achieved between the two methods both in the linear and nonlinear regimes and even under oblique incidence.

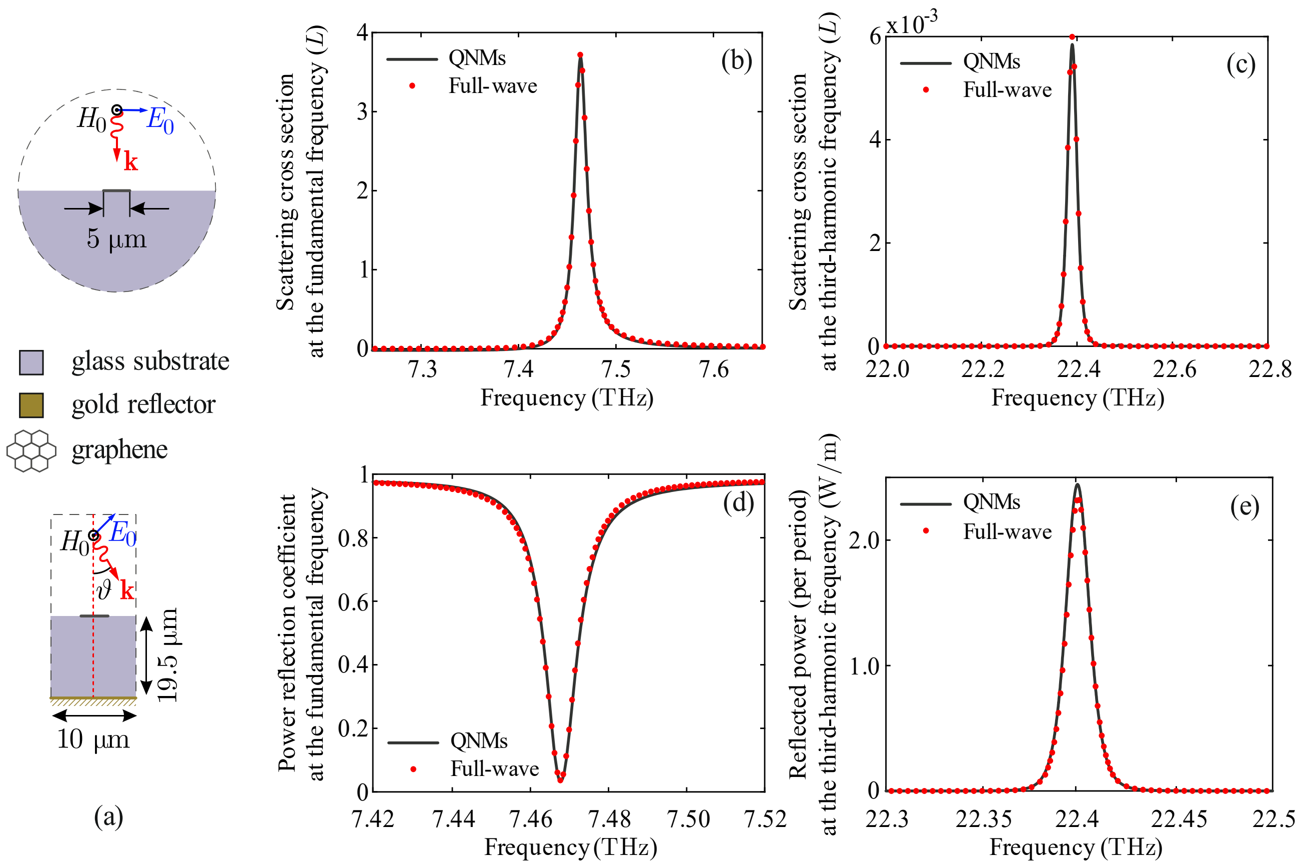

FIGURE 1. (a) The two considered structures comprising graphene on a glass substrate. (b) Linear and (c) nonlinear response (scattering cross-section) of a single graphene strip under normal incidence. (d) Linear and (e) nonlinear response (power reflection coefficient and reflected power, respectively) of a graphene metasurface under oblique incidence (*θ=20º*). QNM expansion (solid lines) and full-wave simulations (red point markers) show excellent agreement in both cases.

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