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A mode coupling model for meta-molecules

B. Vial[1] **and Y. Hao**[1]

[1]School of Electronic Engineering and Computer Science, Queen Mary University of London,
London E1 4NS, United Kingdom
b.vial@qmul.ac.uk

Abstract – **We develop a model for the coupling of leaky eigenmodes in meta-molecules. By expressing the modes of the coupled system as a linear combination of the modes of the isolated meta-atoms, we obtain a generalized eigenvalue problem involving small size dense matrices. We apply this technique to a 2D problem of a high index rod dimmer of rectangular cross section for Transverse Magnetic (TM) polarization. The results of our model are compared with full-wave finite element simulations and show a good agreement for the four lowest eigenvalues by taking into account the two lowest eigenfrequencies of the isolated rods. This model provides interesting physical insights on the coupling scheme at stake in such systems and pave the way for the design and optimization of resonances in more complicated systems, including the engineering of metamaterial unit cells.**

I. Introduction

Metamaterials are a class of material engineered to produce properties that do not occur naturally. Their fundamental building blocks, usually called meta-molecules or meta-atoms, allow to mould the flow of light in an unprecedented way. The study of these individual building blocks is of prime importance since their shape and electromagnetic properties governs the effective behaviour of the metamaterial. In particular, it is of great interest to distinguish which effects arise from the meta-atoms themselves or from their arrangement (periodic or random). We study here the coupling of two individual meta-atoms that form a meta-molecule. Hybridization models have been introduced in the context of plasmonics [1]. The simple and intuitive picture, an electromagnetic analog of molecular orbital theory, describes the plasmon response of complex nanostructures of arbitrary shape as the interaction of plasmons of simpler sub-structures. However, the formalism is limited to the quasistatic approximation.
Coupled mode theories [2, 3] have extensively been studied and applied in particular in the context of optical waveguides. The coupled modes equations are of a heuristic nature and rely upon a slowly varying approximation, thus limiting the domain of application of the method.
The method we develop here is general and relies only on the assumption that the coupled eigenmodes can be expressed as a superposition of the modes of the two uncoupled systems, which can be computed by a suitable numerical method or analytically in some simple cases. It can be applied to arbitrary shaped open resonators with both non trivial (possibly anisotropic) permittivity and permeability. We stress here that it handles *quasi-normal modes* associated with complex eigenvalues [5, 4]. The imaginary part of the eigenfrequency gives the leakage rate of the mode and is fully taken into account in our model. We illustrate the validity of the proposed model on a 2D problem of a high index dimmer of rectangular cross section rods for Transverse Magnetic (TM) polarization. The agreement between the model and full-wave finite element simulations is very good. This model depicts a simple picture allowing a better understanding of the coupled modes in terms of simpler spectral building blocks.

II. Coupled mode model

Consider a system A (material properties $\boldsymbol{\mu}^A$ and $\boldsymbol{\varepsilon}^A$) with eigenvalues $\Lambda_n^A = (\omega_n^A/c)^2$ and non zero eigenvectors $\boldsymbol{E}_n^A$ solution of:

$$\mathcal{M}_{\boldsymbol{\mu}^A}(\boldsymbol{E}_n^A) := \boldsymbol{\nabla}\times\left[(\boldsymbol{\mu}^A)^{-1}\,\boldsymbol{\nabla}\times\boldsymbol{E}_n^A\right] = \Lambda_n^A\,\boldsymbol{\varepsilon}^A\,\boldsymbol{E}_n^A, \tag{1}$$

and a system B (material properties $\boldsymbol{\mu}^B$ and $\boldsymbol{\varepsilon}^B$) with eigenvalues $\Lambda_n^B = (\omega_n^B/c)^2$ and non zero eigenvectors $\boldsymbol{E}_n^B$ such that:

$$\mathcal{M}_{\boldsymbol{\mu}^B}(\boldsymbol{E}_n^B) := \boldsymbol{\nabla}\times\left[(\boldsymbol{\mu}^B)^{-1}\,\boldsymbol{\nabla}\times\boldsymbol{E}_n^B\right] = \Lambda_n^B\,\boldsymbol{\varepsilon}^B\,\boldsymbol{E}_n^B. \tag{2}$$

Now we consider the situation where the two systems A and B are coupled together. For the coupled system denoted C (material properties $\boldsymbol{\mu}^C$ and $\boldsymbol{\varepsilon}^C$), the spectral problem is to find eigenvalues $\Lambda_n^C = (\omega_n^C/c)^2$ and eigenvectors $\boldsymbol{E}_n^C$ such that:

$$\mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_n^C) := \boldsymbol{\nabla}\times\left[(\boldsymbol{\mu}^C)^{-1}\,\boldsymbol{\nabla}\times\boldsymbol{E}_n^C\right] = \Lambda_n^C\,\boldsymbol{\varepsilon}^C\,\boldsymbol{E}_n^C. \tag{3}$$

The only assumption we make here is to consider that the coupled eigenmodes can be written as a linear combination of the modes of the two isolated systems:

$$\boldsymbol{E}_n^C = \sum_i q_{n,i}^A \boldsymbol{E}_i^A + q_{n,i}^B \boldsymbol{E}_i^B \tag{4}$$

Inserting Eq. (4) in the eigenvalue equation (3), and taking into account the linearity of operator $\mathcal{M}_{\boldsymbol{\mu}^C}$ reads:

$$\sum_i q_i^A \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^A) + q_i^B \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^B) = \Lambda_n^C \sum_i q_i^A \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^A + q_i^B \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^B. \tag{5}$$

We denote $\boldsymbol{F}_n^U$ the adjoint eigenvectors (for a problem with Hermitian conjugate material properties) associated with the adjoint eigenvalue $\overline{\Lambda_n^U}$, for $U = \{A, B, C\}$. The eigenmodes and their adjoint satisfies bi-orthogonality conditions [6]:

$$\left\langle \boldsymbol{\varepsilon}^U \boldsymbol{E}_n^U \,\middle|\, \boldsymbol{F}_m^U \right\rangle = \int_\Omega \boldsymbol{\varepsilon}^U(\boldsymbol{r})\,\boldsymbol{E}_n^U(\boldsymbol{r})\cdot\overline{\boldsymbol{F}_m^U}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = K_n^{UU}\delta_{nm}. \tag{6}$$

where the complex-valued normalization coefficient K_n^U is defined as

$$K_n^{UU} := \left\langle \boldsymbol{\varepsilon}^U \boldsymbol{E}_n^U \,\middle|\, \boldsymbol{F}_m^U \right\rangle = \int_\Omega \boldsymbol{\varepsilon}^U(\boldsymbol{r})\,\boldsymbol{E}_n^U(\boldsymbol{r})\cdot\overline{\boldsymbol{F}_n^U}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}. \tag{7}$$

It can in fact been proved that for non periodic problems we have $\overline{\boldsymbol{F}_n^U} = \boldsymbol{E}_n^U$ [5]. Note that we assumed here that the material properties are non dispersive. To take into account dispersion, one should use a modified version of the scalar product defined in Eq.(6) [4].
Projecting Eq. (5) onto adjoint eigenmodes $\boldsymbol{F}_j^A$ and $\boldsymbol{F}_j^B$ reads:

$$\sum_m q_i^A \left\langle \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^A) \,\middle|\, \boldsymbol{F}_j^A \right\rangle + q_i^B \left\langle \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^B) \,\middle|\, \boldsymbol{F}_j^A \right\rangle = \Lambda_n^C \sum_i q_i^A \left\langle \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^A \,\middle|\, \boldsymbol{F}_j^A \right\rangle + q_i^B \left\langle \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^B \,\middle|\, \boldsymbol{F}_j^A \right\rangle$$
$$\sum_m q_i^A \left\langle \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^A) \,\middle|\, \boldsymbol{F}_j^B \right\rangle + q_i^B \left\langle \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^B) \,\middle|\, \boldsymbol{F}_j^B \right\rangle = \Lambda_n^C \sum_i q_i^A \left\langle \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^A \,\middle|\, \boldsymbol{F}_j^B \right\rangle + q_i^B \left\langle \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^B \,\middle|\, \boldsymbol{F}_j^B \right\rangle$$

We denote $Q = (q_i^A; q_i^B)$, $i \in \mathbb{N}$ and

$$N_{ij}^{AA} = \left\langle \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^A) \,\middle|\, \boldsymbol{F}_j^A \right\rangle \qquad N_{ij}^{AB} = \left\langle \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^A) \,\middle|\, \boldsymbol{F}_j^B \right\rangle$$
$$N_{ij}^{BB} = \left\langle \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^B) \,\middle|\, \boldsymbol{F}_j^B \right\rangle \qquad N_{ij}^{BA} = \left\langle \mathcal{M}_{\boldsymbol{\mu}^C}(\boldsymbol{E}_i^B) \,\middle|\, \boldsymbol{F}_j^A \right\rangle$$
$$M_{ij}^{AA} = \left\langle \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^A \,\middle|\, \boldsymbol{F}_j^A \right\rangle \qquad M_{ij}^{AB} = \left\langle \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^A \,\middle|\, \boldsymbol{F}_j^B \right\rangle$$
$$M_{ij}^{BB} = \left\langle \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^B \,\middle|\, \boldsymbol{F}_j^B \right\rangle \qquad M_{ij}^{BA} = \left\langle \boldsymbol{\varepsilon}^C \boldsymbol{E}_i^B \,\middle|\, \boldsymbol{F}_j^A \right\rangle.$$

Denoting also the block matrices

$$N = \begin{pmatrix} N^{AA} & N^{BA} \\ N^{AB} & N^{BB} \end{pmatrix} \qquad \text{and} \qquad M = \begin{pmatrix} M^{AA} & M^{BA} \\ M^{AB} & M^{BB} \end{pmatrix}$$

Moreover, the integrals calculated here converge because they are computed on a finite domain consisting of the actual physical domain surrounded by PMLs [4].
Finding the coupled eigenmodes $\boldsymbol{E}_n^C$ (*i.e.* the expansion coefficients q_i^A and q_i^B) and the coupled eigenvalues Λ_n^C consist in solving a generalized eigenvalue problem

$$N\,Q = \Lambda^C M\,Q \tag{8}$$

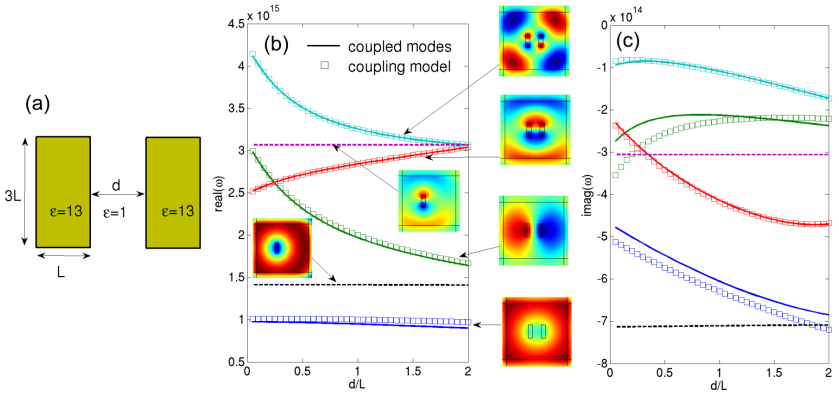

Fig. 1: Setup of the coupled problem (a) and coupled modes computed directly (solid lines) vs. coupling model (squares) as a function of the dimmer gap d. Real (b) and imaginary (c) parts of the associated eigenfrequencies (in Hz). The insets show the field maps $\mathrm{Re}(E_z)$ of the isolated rod modes and the coupled modes for $d/L = 2$.

III. Numerical example

We apply the model to a 2D problem of a dimmer of rods with rectangular cross section embedded in air, with parameters $L = 50$nm, $\varepsilon^{\mathrm{rod}} = 13$, $\mu^{\mathrm{rod}} = 1$ (cf. Fig. 1 (a)) and we study the TM polarization case, i. e. $\boldsymbol{E} = E_z \boldsymbol{e}_z$. The modes of the individual rods are computed with the FEM using Perfectly Matched Layers to truncate the infinite air domain. The lowest frequency mode correspond to the magnetic dipole and the higher frequency mode to the electric dipole along the oriented along the long side of the rod (cf. insets in Fig. 1). We studied the coupling of two identical nanorods as a function of the gap d, by computing directly the dimmer eigenmodes with the FEM and by our model using the two lowest frequency modes of the individual meta-atoms. The results from both methods are in good agreement for both real and imaginary part (cf. Fig. 1 (b) and(c)). The accuracy of our model should be improved by including more leaky modes as well as radiation modes associated with the continuous spectrum of Maxwell's operator [5]. Moreover, the study of the expansion coefficients q_i^A and q_i^B (not shown here) clearly illustrates the the relative contribution of each mode of the individual meta-atoms to the coupled modes as well as the in and out of phase coupling mechanisms.

IV. Conclusion

We have developed a coupled model for computing the eigenmodes of coupled resonators. Its validity is illustrated by the good agreement in comparison to full wave simulations. This model provides physical insights on the coupling of individual modes and should ease the design and understanding of resonant metamaterial unit cells.

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