Modal decomposition of meta-atom dynamics

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Abstract

The modes of meta-atoms are a natural basis for describing their excitation and interaction, however many structures of practical interest are too complex to find their modes analytically. It is shown here how they can be found by solving for the singularities of an integral equation operator. These modes are used to construct simple yet highly accurate models, which are applied here to scattering problems. The proposed technique is implemented in a freely available open source code.

1. Introduction

To understand meta-atoms, nano-antennas or other scattering objects, it is of great benefit to have a simple model which captures all the essential physics of the problem. The most natural way to understand such elements is through their modes. On the basis of these modes, it is possible to understand the coupling processes when resonant particles are brought into proximity to each other [1, 2]. In these works, the modes were approximated by exciting the structure in a regime where it is assumed that only a single mode dominates the response.

Several authors have resorted to dipole moments as a description of the excitation of meta-atoms. Such models can provide an intuitive picture of excitation of meta-atoms in the far-field [3]. However, such an approach can be "over-determined", in the sense that a single mode can have strong contributions from both electric and magnetic dipole moments, thus they are not truly independent degrees of freedom. In addition, higher order modes can be excited, and higher order multipoles may contribute significantly to the response, particularly for near-field interaction effects.

The physical picture of modes as the fundamental degrees of freedom is highly intuitive. However, the concept of a mode is not so well defined for an open system, which radiates energy into the far-field, or dissipates it internally. This means that the operator describing the system is non-Hermitian, the eigenvalues are complex, and the eigenvectors and non-orthogonal.

To solve this problem, first a numerical model of the meta-atoms is created, based on a discretisation of the structure. This forms the basis of a matrix description created using the method of moments [4] integral technique. The modes of the system correspond to the complex frequencies at which this matrix becomes singular, with the modal distribution given by the latent vectors [5]. The code used to calculate the results presented here has been publicly released under an open source license [9].

2. Model

Since this model involves analytical extension of the frequency into the complex plane, it is most convenient to consider all quantities to have an implicit time dependence of $\exp(st)$ with $s = \Omega + j\omega$, whereby spectral quantities are related to time domain via a two-sided Laplace transform pair. The description of the system begins with the electric field integral equation, describing the scattered field produced by a system of currents:

$$\mathbf{E}_s\left(\mathbf{r}, s\right) = \int \overline{\overline{G}}(\mathbf{r} - \mathbf{r}', s) \cdot \mathbf{j}(\mathbf{r}', s) \mathrm{d}\mathbf{r} \tag{1}$$

In the most general case, this includes both conduction currents in metals, and polarisation currents in dielectrics. The dyadic Green's function $\overline{\overline{G}}$ describes the electric field produced by a current element. In free space, it is given by:

$$\overline{\overline{G}}\left(\mathbf{r}\right) = \left[-s\mu\overline{\overline{I}} + \frac{1}{s\epsilon}\nabla\nabla\right] \frac{\exp(-jk_0|\mathbf{r}|)}{4\pi|\mathbf{r}|} \tag{2}$$

For the simplest case of perfectly conducting metals, the scattered field $\mathbf{E}_s$ can be related to the incident field $\mathbf{E}_i$ through the requirement that the tangential components cancel out on the surface $\hat{\mathbf{n}} \times \mathbf{E}_i = -\hat{\mathbf{n}} \times \mathbf{E}_s$

The procedure begins by creating a triangular mesh on the surface of the geometry, allowing arbitrary shaped meta-atoms to be described. In the following description, a split-ring resonator is used, represented as an infinitesimally thin metallic layer. N basis functions are constructed over the mesh, which represent both the incident field and the induced current.

The result is a matrix equation which describes the full dynamics in discretised form:

$$\mathrm{V}(s) = \mathrm{Z}(s) \cdot \mathrm{I}(s) \tag{3}$$

where V is a vector of length N describing the incident field, I is also of length N and describes the induced currents, whilst Z is the $N \times N$ impedance matrix which relates the two.

3. Determining the modes

The modes of a system are solutions which satisfy the relevant equations in the absence of a driving source term. In

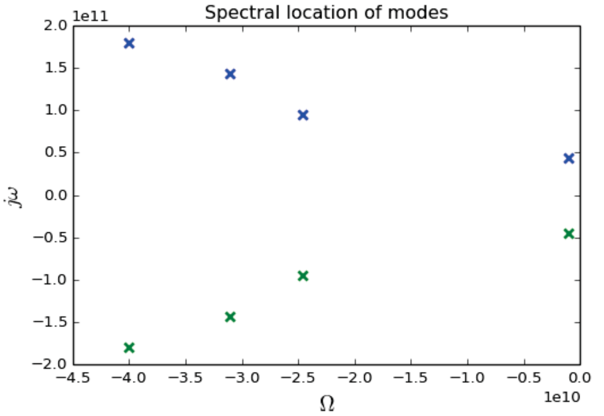

Figure 1: The singularities of the operator in the s-plane, which correspond to the resonant frequencies.

the context of Eq. (3), this involves solutions to the homogeneous problem $\mathrm{Z} \cdot \mathrm{I} = 0$. However, for an open radiating system, the matrix Z is non-Hermitian, therefore such solutions cannot be found for real frequencies (represented by imaginary values of s in this notation). Therefore, it is necessary to search for complex values of s which satisfy this condition. Since the matrix Z has explicit dependence on s, the problem is nonlinear in s and must be solved using iterative methods [5]. Linearising the eigenvalue problem provides robust initial estimates for the modes, which are required for the iterative procedure to converge.

The values of s satisfying the inhomogeneous equation are known as the latent values [5]. In Fig. 1 they are shown for the first four modes of a split ring resonator. It can be seen that the higher order modes are further away from the imaginary s axis, indicating that they have stronger radiative losses. Additionally, these singularities occur in complex-conjugate pairs, as required for the system response to be a real-function when expressed in the time domain.

For each latent value s_n corresponding to the resonant frequency a mode, there is a latent vector I_n which satisfies the homogeneous equation. These vectors give the current distributions of the modes, which are shown in Fig. 2 for a split ring resonator. The arrows give the distribution of surface current, whilst the colours show the corresponding surface charges.

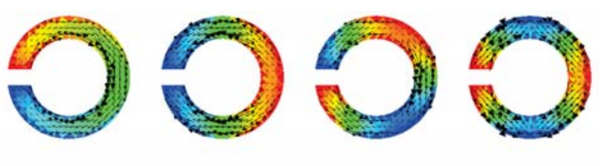

Figure 2: The first four modes of a split ring resonator

As expected, the higher order modes show more nodes and anti-nodes in their distribution. An important point is that these modes have been found *independent of any excitation*. Thus we can be certain that they represent the most basic degrees of freedom of the meta-atom. This is in contrast to the more common approach of illuminating a structure and observing the current distribution at a peak of scattering, which may yield some arbitrary superposition of modes. In addition, searching for complex singularities also reveals dark modes which may not be excited for a given polarisation of the incident wave.

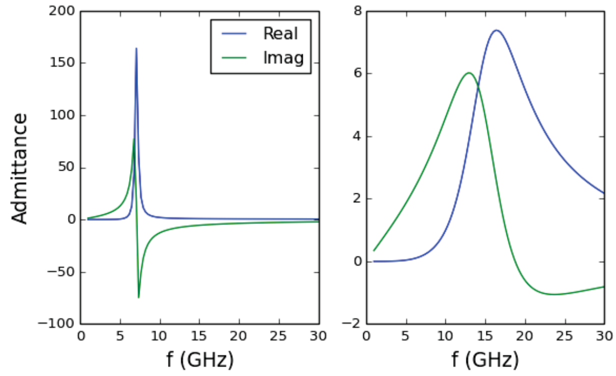

Figure 3: The scalar admittance functions for the first two modes of the SRR

4. Broadband model

The main motivation for finding the modes is to enable a simple and intuitive model to be constructed from a complex, fully-numerical one. At a fixed frequency s, it is possible to decompose the impedance matrix in terms of its eigenvalues and eigenvectors:

$$\mathrm{Z}(s) = v(s) \cdot z(s) \cdot v^T(s) \tag{4}$$

where $z(s)$ is a diagonal matrix containing the eigenvalues and the n columns of $v(s)$ are the eigenvalues of Z. The appearance of v twice in Eq. (4) is due to Z being complex-symmetric (i.e. $\mathrm{Z} = \mathrm{Z}^T$). This is known as the Eigenvalue Expansion Method [6], and has been successfully applied to antenna arrays [7], and more recently to plasmonic structures [8]. We see that an arbitrary current is projected as a sum of eigenvectors, each of which has some scalar impedance imposed on it by the corresponding mode.

While Eq. (4) reduces a large matrix equation to a scalar model, it is desirable to develop a single model which is accurate over a wide frequency range, rather than filling and factoring the impedance matrix at every frequency. With the Singularity Expansion Method [6], we can use the singularities in the s plane to construct a wideband model. By numerically determining $\mathrm{d}z_n/\mathrm{d}s$ at $s = s_n$, and enforcing the impedance to be open-circuit at $s = 0$, a fourth order polynomial is fitted to each scalar impedance z_n. The additional assumption is made that $v(s) \approx v(s_n)$, which is found to be quite accurate for several structures of practical interest.

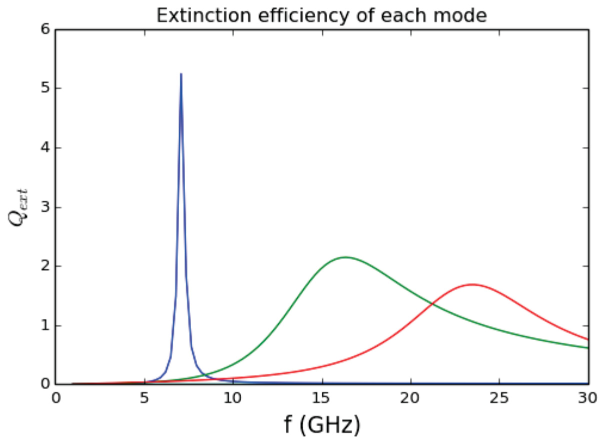

Figure 4: The extinction efficiency of each mode

The eigendecomposition is quite useful when solving the dynamics of the structure. In particular, the excited current can be found from:

$$\mathrm{I}(s) = \mathrm{Z}^{-1}(s) \cdot \mathrm{V}(s) = \sum_{n=1}^{N} \frac{1}{z_n(s)} v_n \left(v_n \cdot V(s) \right) \quad (5)$$

In practice, the summation only needs to include a few modes which contribute to the dynamics at a particular frequency. In Fig. 3 the scalar admittances $z_n^{-1}(s)$ are shown for the first two modes of a split ring resonator. The resonant behaviour is clearly observable, and is very similar to a series RLC circuit.

5. Extinction calculations

The accurate determination of the mode currents, along with the broadband model, are applicable to almost any problem involving meta-atoms, such as hybridisation of coupled resonators, Fano interference effects, and also to other areas such as nano-antennas. Perhaps the simplest phenomenon to model is scattering, which is addressed here.

The extinction cross-section represents the total power which a scatterer extracts from the incident field through the processes of scattering or absorption. It is given by $\sigma_{ext} = \Re\{\mathrm{V}^* \cdot \mathrm{I}\}$, and is normalised to the physical area of the scatterer in order to yield an efficiency Q_{ext}.

Here, extinction is calculated for an SRR, excited by a plane-wave parallel to its central axis, polarised with the electric field across the gap. In Fig. 4, the first four terms of Q_{ext} are shown, calculated from Eq. (5). The fourth mode has no contribution for this frequency range and choice of incident field. The sum of these contributions is found to agree very well with the directly calculated extinction, and is quicker to calculate by around 2 orders of magnitude. It can be seen that for higher frequencies, a superposition of modes is simultaneously excited.

6. Conclusions

A modal decomposition of the dynamics of small resonant scatterers was presented. This procedure uses an accurate numerical model to derive a simplified scalar model, which is of great benefit for solving problems involving many interacting elements. By searching for singularities, modes can be determined in a manner which is independent of any excitation, and which allows the total response to be found from the contribution of multiple modes. A python code implementing this method is available from [9].

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