Calculating Scattering Spectra using Time-domain Modeling of Time-modulated Systems

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Abstract—Obtaining agreement between theoretical predictions that assume single-frequency excitation and finite-difference time-domain (FDTD) simulations that employ broadband excitation in the presence of time-varying materials is challenging due to frequency mixing. A simple solution is proposed to reduce artifacts in FDTD-calculated spectra from the frequency mixing induced by harmonic refractive index modulation applicable to scenarios in which second order and higher harmonics are negligible. Advantages of the proposed method are its simplicity and applicability to arbitrary problems including resonant structures.

Index Terms—cavity resonators, finite-difference time-domain method, time-varying circuits.

I. INTRODUCTION

The finite-difference time-domain method (FDTD) can generate entire scattering spectra in a single simulation run by exciting the system with a broadband source. The scattering parameters are calculated by dividing the scattered power spectrum by the incident power spectrum. However, in the case of time-modulated systems, one must exercise caution when calculating the scattering coefficients by dividing the scattered power by the incident power due to the frequency mixing caused by the modulation. Here, we explore the severity of this problem by comparing FDTD simulation results to theoretical predications, and we propose a simple solution to improve the agreement between theory and simulation in time-modulated systems. This problem has been previously addressed in the context of scattering from space-time modulated metasurfaces [1]; however, extension of that technique to resonant structures such as those analyzed here has not yet been reported. An advantage of the approach reported here is its simplicity, requiring only two executions of a standard pulse scattering simulation and minimal post-processing.

II. COUPLED MODE ANALYSIS OF MODULATED SYSTEM

Fig. 1 (a) illustrates the coupling of two generic resonators that are each coupled to a waveguide. Fig. 1 (b) shows the system geometry that was simulated using FDTD. Of particular interest is the modulation of the refractive index via the electrooptic effect and an applied voltage. Modulating the refractive indices of the cavities introduces a small signal perturbation to the resonance frequency $\omega_0 + \delta\omega \cos(\omega_m t)$ where $\delta\omega$ is the change in resonance frequency due to the refractive index change. In another presentation [2] we show how the system can be designed to transmit near unity power at the resonance frequencies of the coupled cavities $(\omega_0 \pm \kappa)$ when the modulation is off $(\delta \omega = 0)$ and to reduce transmission to less than 1% when the modulation is applied as shown in Fig. 1 (b).



Fig. 1. (a) Generic depiction of two coupled resonant cavities each of which is coupled to a waveguide. ω_0 is the resonance frequency of an isolated resonator. κ is the coupling rate between the two cavities. *d* is the coupling rate between one cavity and one waveguide. (b) Depiction of the system modeled using FDTD. (c)-(f) Comparison between CMT and FDTD results: (c) when there is no applied modulation; (d) in the presence of modulation with normalized modulation frequency $\omega_m = 0.005$ and amplitude $\delta\omega = 0.0031$; (e) in the presence of modulation and a multi-frequency CMT model is used; (f) when the first order harmonics are canceled from the FDTD results.

Working in the coupled-cavity basis, the coupled mode theory (CMT) equations describing the dynamics of the system in Fig. 1 (a) are given by $\dot{\mathbf{a}} = [-i\mathbf{\Omega} - i\delta\mathbf{\Omega}(t) - \mathbf{\Gamma}]\mathbf{a} + \sqrt{2}\mathbf{D}^{\mathrm{T}}\mathbf{s}_{\mathrm{inc}}$ where $\mathbf{a} = \begin{bmatrix} a_{+}(t) & a_{-}(t) \end{bmatrix}^{T}$ represents the energy in the even (+) and odd (-) coupled cavity modes, $\mathbf{\Gamma}$ is a diagonal matrix

with γ on the diagonal, Ω is given by:

$$\mathbf{\Omega} = \begin{bmatrix} \omega_0 + \kappa & 0\\ 0 & \omega_0 - \kappa \end{bmatrix},\tag{1}$$

and

$$\mathbf{D} = \frac{1}{\sqrt{2}} \begin{bmatrix} d & d \\ d & -d \end{bmatrix}.$$
 (2)

d is the coupling rate between the cavity and the waveguide. $\mathbf{s}_{inc} = \begin{bmatrix} s_{i1} & s_{i2} \end{bmatrix}^T$ is a vector describing the incident field amplitudes in ports 1 and 2 [3]. In the presence of waveguide coupling, the loss rate decomposes into $\gamma = \gamma_i + \gamma_c$ where γ_i is the intrinsic cavity loss rate, and γ_c is the loss rate due to cavity coupling. The loss rate is related to the waveguide coupling parameter *d* via $d^2 = 2\gamma_c$. In the coupled-cavity basis $\delta \mathbf{\Omega}(t)$ is given by:

$$\delta \mathbf{\Omega}(t) = \begin{bmatrix} 0 & \delta \omega \cos(\omega_m t) \\ \delta \omega \cos(\omega_m t) & 0 \end{bmatrix}.$$
 (3)

The scattered wave amplitude into ports 1 and 2 is determined using $\mathbf{s}_{ref} = -\mathbf{s}_{inc} + \mathbf{D}\mathbf{a}$ where $\mathbf{s}_{ref} = \begin{bmatrix} s_{r1} & s_{r2} \end{bmatrix}^{T}$ represents the amplitudes of the outgoing waves in ports 1 and 2 [3].

To solve the CMT equations, one must introduce the ansatz $a_{\pm}(t) = \sum_{n} a_{\pm,n} e^{-i(\omega + n\omega_m)t}$ and solve for the Fourier series coefficients $a_{\pm,n}$. The equations governing $a_{\pm,n}$ are:

$$[-i(\omega + n\omega_m - w_0 - \kappa) + \gamma]a_{+,n} + \frac{\delta\omega}{2}(a_{-,n+1} + a_{-,n-1}) = ds_{i1}\delta_{n,0},$$
(4)

and

$$[-i(\omega + n\omega_m - w_0 + \kappa) + \gamma]a_{-,n} + \frac{\delta\omega}{2}(a_{+,n+1} + a_{+,n-1}) = ds_{i1}\delta_{n,0},$$
(5)

assuming incidence from port 1. Exact solutions to these equations do not exist, so the Fourier series must be truncated. We discovered that the solution for $a_{\pm,n} \sim (\delta \omega)^n$. So if $\delta \omega \ll \omega_0$, then keeping only the first order harmonics n = -1, 0, 1 is justified.

III. TIME-MODULATED CAVITIES

Fig. 1 (c) displays the reflection $(|S_{11}|^2)$ and transmission $(|S_{21}|^2)$ coefficients determined using FDTD when no modulation is applied to the cavities ($\delta \omega = 0$). The system is excited by a broadband pulse in port 1. The incident and scattered powers are measured in ports 1 and 2. The plot shows significant power transmission at the coupled-cavity resonances ($\omega_0 \pm \kappa$) but little transmission at other frequencies. The agreement between the CMT results and the FDTD results is good. Fig. 1 (d) shows the scattering spectra when the modulation is applied, and less agreement between the CMT and FDTD results is observed. The reason for this disagreement is that the system is excited by a continuous range of frequencies; whereas, the CMT model assumes excitation by a single frequency. To confirm this hypothesis, we can remove the delta functions in Eqs. 4 and 5 which introduces input



Fig. 2. Comparison between CMT and FDTD using the odd-order harmonic cancelation scheme. (a) and (c) change the modulation frequency while keeping $\delta \omega = 0.0031$. (b) and (d) change the modulation amplitude while keeping $\omega_m = 0.005$.

energy at all harmonic frequencies $\omega + n\omega_m$. The result is shown in Fig. 1 (e) where the agreement between CMT and FDTD results is improved.

Returning to the observation that $a_{\pm,n} \sim (\delta \omega)^n$, we surmised that if two FDTD simulations are run where the first is run normally, and then a second is run with $\delta \omega \rightarrow -\delta \omega$ and the scattering spectra of the two are added, then the odd-order harmonics will be filtered out. Fig. 1 (f) depicts the comparison of FDTD results obtained in this manner with CMT calculations assuming single-frequency excitation showing good agreement.

The technique of running two FDTD simulations with the sign of the perturbation reversed is applicable only when the contributions from $a_{\pm,\pm 1}$ are the dominant terms causing disagreement between single-frequency CMT and pulsed excitation FDTD. Fig. 2 explores regions of validity of this assumption. Figs. 2 (a) and (c) consider modulation frequencies $\omega_m = 0.003$ and 0.007. As the modulation frequency increases, the interference from uncanceled second order harmonics decreases and the agreement improves. Figs. 2 (b) and (d) consider $\delta\omega$ values 0.0055 and 0.0016. As the modulation modulation amplitude decreases, the interference from uncanceled second order harmonics decreases and the agreement improves.

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