Convergence Analysis of Padé Interpolation for Extracting Large Quality Factors in Photonic Crystal Double Heterostructure Resonant Cavities

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Abstract—The number of time steps required for accurate estimation of quality factors using Padé interpolation for photonic crystal double heterostructures is investigated. Use of different orders of Padé polynomials is also discussed, and an improvement in convergence is observed as the order of the denominator polynomial is increased.

I. INTRODUCTION

Recently the photonic crystal double heterostructure (PCDH) has received considerable attention due to its small size and high quality factor ($Q$) which can exceed $10^6$ [1], [2]. In this work we investigate the convergence of the Padé interpolation method to extract such large $Q$ values as well as the effect of small frequency separation between resonances in these cavities.

FDTD explicitly discretizes the Maxwell curl equations on a spatial grid and performs a discretized temporal update [3]. A time record of the field evolution may be stored in memory for various spatial points, and the resulting time sequence may be analyzed to obtain resonance frequencies and rates of energy loss out of the cavity. Because photonic crystal devices consist of subwavelength variation in the dielectric constant, fine spatial discretization is required. Furthermore, a stability condition constrains the size of the time step to a value determined by the spatial discretization making long time evolution computationally intensive. Discrete Fourier transforms (DFT) are often used to analyze the spectral content of the resulting time sequences. Because the frequency resolution of a DFT is inversely proportional to the length of the time sequence, long time sequences are preferable to obtain convergence in the spectral features. The quality factor is determined by measuring the full width at half maximum of the resonance peak. The highest resolvable $Q$ from the raw spectral data for a FDTD run with $10^4$ to $10^5$ time steps is on the order of 1000. To overcome this limited resolution several techniques are available including filter-diagonalization[4], Prony’s method[5] and Padé interpolation[6], [7]. In this paper, we investigate the convergence of the Padé interpolation to estimate $Q$ in photonic crystal double heterostructure resonant cavities for different orders of the fitting polynomials. We also investigate the dependence of $Q$ and free spectral range on the number of time steps required for acceptable convergence.

II. PADÉ INTERPOLATION METHOD

The Padé interpolation method fits raw DFT spectral data to a ratio of polynomials defined in Eq. (1).

$$
P(M, N) = \frac{a_0 + a_1\omega + \ldots + a_M\omega^M}{b_0 + b_1\omega + \ldots + b_N\omega^N}
$$

(1)

The temporal evolution of a resonance mode follows a damped sinusoid whose Fourier transform is a Lorentzian. The functional form of a Lorentzian is

$$
\frac{A}{\omega_0/2Q - i(\omega - \omega_0)}
$$

(2)

which indicates that a Padé function $P(0, 1)$ is the correct functional form. Fig. 1(a,) displays the convergence of $Q$ as a function of number of time steps used in the DFT for three different values of $Q$. The Padé interpolation was applied to the DFT of an artificially generated time sequence representing...
In this case we use \( P(3, 2) \). Furthermore, the denominator polynomial is factored into the product of two first order polynomials, and the overall Padé function is written as the sum of two terms with first order polynomials in the denominators. One of these terms will be the dominant term for the resonance under study. The resonance under study has \( Q = 10^6 \), and the neighboring resonance has \( Q = 10^5 \). One sees that with 50,000 time steps frequency spacing between resonances should be greater than 0.001 in normalized frequency \( \Delta f \) which is consistent with the frequency resolution of \( \Delta f = 0.0008 \). Going to 100,000 time steps, one observes that \( Q \) stabilizes after the resonances are separated by only 0.0001 in normalized frequency which is below the DFT frequency resolution.

III. PHOTONIC CRYSTAL DOUBLE HETEROSTRUCTURE RESONANT CAVITIES

Fig. 2(a) displays a schematic illustration of a PCDH. A bound state is formed by perturbing the lattice constant of a few holes in an otherwise uniform photonic crystal waveguide. In Fig. 2(b), we show the raw spectral data obtained from a DFT of a 200,000 time step sequence. The simulated device has 20 uniform photonic crystal waveguide periods on either side of the perturbation which is discretized on a 950 x 340 x 200 grid and parallelized on about 100 processors. The time record required about 20 hours of computation. The spectrum shows a large peak near \( \omega a / 2\pi c = 0.265 \) and some smaller peaks slightly higher in frequency. The high-\( Q \) nature of the resonance combined with the close proximity of the neighboring peaks make accurate analysis of these structures challenging.

In Fig. 3(a-c) we investigate the convergence of \( Q \) as a function of time steps used in the DFT for different Padé polynomials. For this structure \( \alpha' = 1.05\alpha \). It is apparent that the number of time steps required for a stable \( Q \) value is reduced as the order of the denominator polynomial is increased. We stop at \( N = 4 \) as one cannot use algebraic methods to factor the denominator polynomial for \( N > 4 \). Finally in Fig. 3(d) we test convergence of \( Q \) for different lattice constant perturbations. As the lattice constant is increased the \( Q \) decreases, and the frequency separation increases allowing for faster convergence. In addition, the \( Q \) of 5% perturbation structure with a lower dielectric substrate is investigated. In the lower three curves, a stable \( Q \) value is obtained after about 50,000 time steps.

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