Extracting Large Quality Factors in Photonic Crystal Double Heterostructure Cavities Using the Padé Method

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High quality factor photonic crystal cavities

D1 cavity, $Q \sim 10^6$

L3 cavity, $Q \sim 10^5$

PCDH cavity, $Q \sim 10^6\text{-}10^9$

H. Y. Ryu, M. Notomi, Y. H. Lee
Appl. Phys. Lett. 83 4294 2003

Y. Akahane, T. Asano, B.-S. Song, S. Noda
Nature 425 944 2005

B.-S. Song, S. Noda, T. Asano,
Y. Akahane
Nature Materials 4 207 2005

| Biological and chemical sensors |
| Slow light (optical memory and buffers) |
| Lasers and filters for chip-scale photonic integration |
Photonic crystal double heterostructure lasers and cavities

>100μW edge-emitting output power

bound state formation near dispersion extrema

CLEO paper CMV3 (2007).

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Presentation outline

Finite-Difference Time-Domain numerical simulation technique

Optical loss in photonic crystal resonant cavities

Discrete Fourier transform + Padé interpolation method for quality factor estimation

Application to photonic crystal double heterostructure cavities
Finite-difference time-domain analysis of photonic crystal resonant cavities

Discretized spatial derivatives

\[
\frac{\partial D_x^{i, j+1/2, k+1/2}}{\partial t} = \frac{1}{\Delta y} \left( H_z^{i, j+1, k+1/2} - H_z^{i, j, k+1/2} \right) - \frac{1}{\Delta z} \left( H_y^{i, j+1/2, k+1} - H_y^{i, j+1/2, k} \right)
\]

\[
\frac{\partial B_x^{i-1/2, j+1, k+1}}{\partial t} = \frac{1}{\Delta z} \left( E_y^{i-1/2, j+1, k+3/2} - E_y^{i-1/2, j+1, k+1/2} \right) - \frac{1}{\Delta y} \left( E_z^{i-1/2, j+3/2, k+1} - E_z^{i-1/2, j+1/2, k+1} \right)
\]

Discretized time derivatives

\[
\frac{\partial D_x^{i, j+1/2, k+1/2}}{\partial t} = \left[ \varepsilon \frac{E_x^{n+1/2} - E_x^{n-1/2}}{\Delta t} \right]^{i, j+1/2, k+1/2}
\]

\[
\frac{\partial B_x^{i-1/2, j+1, k+1}}{\partial t} = \left[ \mu \frac{H_x^{n+1} - H_x^n}{\Delta t} \right]^{i-1/2, j+1, k+1}
\]

FDTD simulation parameters

\[
\Delta t \leq \frac{\Delta x}{c \sqrt{3}} \quad \Delta t = 0.87 \frac{\Delta x}{c \sqrt{3}}
\]

\[
\Delta x = \frac{a}{20} \quad \text{Effectively 40 samples per lattice constant}
\]
Numerical analysis method

- Broadband initial condition to excite all cavity resonances
- Propagate the fields in time for $10^5$ FDTD time steps
- 15 layers of PML on all boundaries to absorb leaky radiation from the cavity
- Spectral analysis using discrete Fourier transform on resulting time sequence
Photonic crystal double heterostructure resonant cavities

\[ \omega \]

\[ H_z(x,y) \]

20 PCWG periods each side
8 PC rows top and bottom

Computational resources
950 x 340 x 200 spatial points
100 processors
20 hours for 200k time steps
Photonic crystal double heterostructure: Free spectral range

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$H_z(x, y)$
Leakage mechanisms in PCDH cavities

Out-of-plane: wavevector components not totally internally reflected
In-plane: finite number of photonic crystal cladding periods
           finite number of photonic crystal waveguide periods

\[ \frac{P(\text{out-of-plane})}{P(\text{in-plane})} = 1.8 \]
\[ \frac{P(\text{waveguide})}{P(\text{pc cladding})} = 0.2 \]

20 PCWG periods each side
8 PC rows top and bottom
Methods of calculating the quality factor

- Physical definition of $Q$

$$Q = \omega_0 \frac{\langle U \rangle}{\langle \frac{dU}{dt} \rangle}$$

- Damped cosine time function (Filter Diagonalization)

$$f[n] = f_0 e^{-\omega_0 n \Delta t / 2Q} \cos(\omega_0 n \Delta t)$$

- Fourier transform is a Lorentzian function (Padé interpolation)

$$F(\omega) = \frac{f_0 / 2}{\omega_0 \frac{\omega_0}{2Q} - i(\omega - \omega_0)}$$

$$Q = \frac{\omega_0}{\Delta \omega}$$
Discrete Fourier transform resolution

\[ \Delta f = \frac{1}{N \Delta t} \]

\[ f[n] = f_0 e^{-\omega_0 n \Delta t / 2Q} \cos(\omega_0 n \Delta t) \]
Discrete Fourier transform resolution

$Q = 10000$

amplitude decreased to 0.98 after 10k time steps
Padé interpolation method

\[
\begin{align*}
\frac{\alpha_0 + \alpha_1 \omega_s + \alpha_2 \omega_s^2 + \ldots + \alpha_M \omega_s^M}{\beta_0 + \beta_1 \omega_s + \beta_2 \omega_s^2 + \ldots + \beta_N \omega_s^N} &= \frac{Q_M(\omega_s)}{D_N(\omega_s)} = F(\omega_s) \\
\end{align*}
\]

where \( \omega_s = s \Delta \omega \) is the \( s \)th DFT frequency sample

setting \( \beta_0 = 1 \) and multiplying both sides by the denominator yields

\[
\begin{align*}
\alpha_0 + \alpha_1 \omega_s + \alpha_2 \omega_s^2 + \ldots + \alpha_M \omega_s^M &= F(\omega_s)(1 + \beta_1 \omega_s + \beta_2 \omega_s^2 + \ldots + \beta_N \omega_s^N) \\
\alpha_0 + \alpha_1 \omega_s + \alpha_2 \omega_s^2 + \ldots + \alpha_M \omega_s^M - F(\omega_s)(\beta_1 \omega_s + \beta_2 \omega_s^2 + \ldots + \beta_N \omega_s^N) &= F(\omega_s) \\
\end{align*}
\]

M+1 \( \alpha \)-terms and N \( \beta \)-terms

linear equation with M+N+1 unknowns which requires M+N+1 DFT frequency samples for a unique solution

Padé interpolation method for Lorentzian lineshapes

General Padé function

\[
P(M,N) = \frac{Q_M(\omega_s)}{D_N(\omega_s)} = \frac{\alpha_0 + \alpha_1 \omega_s + \alpha_2 \omega_s^2 + \ldots + \alpha_M \omega_s^M}{\beta_0 + \beta_1 \omega_s + \beta_2 \omega_s^2 + \ldots + \beta_N \omega_s^N}
\]

Damped cosine time function has Lorentzian function Fourier transform

\[
f(t) = f_0 e^{-\omega_0 t/2Q} \cos(\omega_0 t) \quad \leftrightarrow \quad F(\omega) = \frac{f_0/2}{\omega_0/2Q - i(\omega-\omega_0)}
\]

Padé function corresponding to Lorentzian form

\[
P(0,1) = \frac{\alpha_0}{1 + \beta_1 \omega} = \frac{-i \alpha_0 / \beta_1}{-i/\beta_1 - i \omega} = \frac{-i \alpha_0 / \beta_1}{-i/\beta_1 - i \omega_0 - i(\omega-\omega_0)}
\]

\[
-i/\beta_1 - i \omega_0 = \frac{\omega_0}{2Q}
\]
Padé convergence – user defined time sequence

\[-i/\beta_i - i\omega_0 = \frac{\omega_0}{2Q}\]

\[1/\beta_i + \omega_0 = i \frac{\omega_0}{2Q}\]

Complex number \rightarrow Real number \rightarrow Imaginary number

\[\text{Re}\{1/\beta_i\} = -\omega_0\]

\[\text{Im}\{1/\beta_i\} = \frac{\omega_0}{2Q}\]

\[Q = \frac{-\text{Re}\{1/\beta_i\}}{2\text{Im}\{1/\beta_i\}}\]

Quality Factor (Q)

Time Step (x1000)

Q = 10^6
Q = 10^5
Q = 10^4
For $P(0,1)$, the Padé method requires $M+N+1 = 0 + 1 + 1 = 2$ DFT frequency samples for a unique solution

For $P(1,1)$, the Padé method requires $M+N+1 = 1 + 1 + 1 = 3$ DFT frequency samples for a unique solution

\[ P(1,1) = \frac{\alpha_0 + \alpha_1 \omega}{1 + \beta_1 \omega} = \frac{\alpha_1}{\beta_1} + \frac{\alpha_0 - \alpha_1 / \beta_1}{1 + \beta_1 \omega} \]

\[ \text{Re}\{1/\beta_1\} = -\omega_0 \]
\[ \text{Im}\{1/\beta_1\} = \frac{\omega_0}{2Q} \rightarrow Q = \frac{-\text{Re}\{1/\beta_1\}}{2\text{Im}\{1/\beta_1\}} \]
For \( P(0,1) \), the Padé method requires
\[ M+N+1 = 0 + 1 + 1 = 2 \]
DFT frequency samples for a unique solution.

For \( P(1,1) \), the Padé method requires
\[ M+N+1 = 1 + 1 + 1 = 3 \]
DFT frequency samples for a unique solution.

\[
P(1,1) = \frac{\alpha_0 + \alpha_1 \omega}{1 + \beta_1 \omega} = \frac{\alpha_1}{\beta_1} + \frac{\alpha_0 - \alpha_1 / \beta_1}{1 + \beta_1 \omega}
\]

\[
\text{Re}\{1/\beta_1\} = -\omega_0
\]
\[
\text{Im}\{1/\beta_1\} = \frac{\omega_0}{2Q} \quad \rightarrow \quad Q = \frac{-\text{Re}\{1/\beta_1\}}{2\text{Im}\{1/\beta_1\}}
\]
Padé convergence – user defined time sequence with two resonances

\[ P(2,2) = \frac{\alpha_0 + \alpha_1 \omega + \alpha_2 \omega^2}{1 + \beta_1 \omega + \beta_2 \omega^2} = \frac{\alpha_2}{\beta_2} \left( \frac{\alpha_0 + \alpha_1 - \frac{\alpha_2}{\beta_2} \omega}{1 + \beta_1 \omega + \beta_2 \omega^2} \right) \]

\[ P(2,2) = \frac{\alpha_2}{\beta_2} + \frac{C_1}{\frac{\omega_1}{2Q_1} - i(\omega - \omega_1)} + \frac{C_2}{\frac{\omega_2}{2Q_2} - i(\omega - \omega_2)} \]
Padé convergence – FDTD analyzed PCDH cavity

- 10k time step transient removed
- Converged $Q = 336.7k$
- $< 1\%$ fluctuation in the unshaded portion
- 10k transient + 50k for $P(3,3)$, $P(3,4)$, $P(4,4)$
Verification of $Q$ value using complementary methods

Explicit calculation

\[ f[n] = e^{-\omega_0 n \Delta t / 2Q} \]

\[ Q = \omega_0 \frac{\langle U \rangle}{\langle \frac{dU}{dt} \rangle} \]

Padé $Q = 336.7k$

Energy density $Q = 329.3k$
Comparison between Padé and filter diagonalization method

Filter-Diagonalization


ab-initio.mit.edu/harminv/
Summary

FDTD analysis of PCDH cavities
Time sequence length – spectral resolution
Convergence properties of different Padé functions
Application to photonic crystal double heterostructure cavities

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