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Application of Padé Approximation in Simulating Photonic Crystals *

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Abstract: To save finite-difference time-domain (FDTD) computing time, several methods are proposed to convert the time domain FDTD output into frequency domain. The Padé approximation with Baker's algorithm and the program are introduced to simulate photonic crystal structures. For a simple pole system with frequency 160THz and quality factor of 5000, the intensity spectrum obtained by the Padé approximation from a 2^8-item sequence output is more exact than that obtained by fast Fourier transformation from a 2^{20}-item sequence output. The mode frequencies and quality factors are calculated at different wave vectors for the photonic crystal slab from a much shorter FDTD output than that required by the FFT method, and then the band diagrams are obatined. In addition, mode frequencies and Q-factors are calculated for photonic crystal microcavity.

Key words: optical waveguides; photonic bandgap; photonic crystal; microcavity; finite-difference time-domain
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1 Introduction

The finite-difference time-domain (FDTD) technique[1] is widely used to simulate optical microcavities and photonic crystal because it can deal with complex cavity structures flexibly[2~7]. However, the FDTD simulation only yields the time variation of electromagnetic fields, i.e. the FDTD output. The FDTD output must be transformed into frequency-domain to obtain mode frequencies and quality factors. The common selection to use is the fast Fourier transform (FFT) method, which has resolution inversely proportional to the total persistence time of the FDTD iteration, i.e. the product of the iteration number and the time step. The time step of the FDTD simulation is limited by the Courant limit, so a very large FDTD iteration number is required when a high-quality-factor mode exists or several modes have nearly degenerate frequencies, which always means a terrible computation task. To save the computing time of the FDTD process, Prony's method[8], the matrix-pencil method[9], and the FFT/Padé approximation method[10] have been used to efficiently analyze the FDTD output. Recently, we apply a Padé approximation with Baker's algorithm[11] for calculating the mode frequencies and quality factors[12], and find that the method is easy to manipulate and can save more computation time than the FFT/Padé approximation, especially for a cavity with nearly degenerate modes.

In this paper, we apply the Padé approximation with Baker's algorithm to evaluate the mode frequencies and quality factors from the FDTD output for photonic crystals and a photonic crystal microcavity and compare the results with those obtained by the FFT method. The results show that the FFT method cannot yield accurate mode quality factors even using a 32 times longer FDTD output

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than that of the Padé approximation. Suppressing the spectral width of the impulse function to excite only one mode, we analyze the single mode field varying with time and calculate its resonant frequency and quality factor, and thus obtain the results well in agreement with those obtained by the Padé approximation. We also calculate the mode frequencies and quality factors at different wave vectors, obtain the band diagrams for photonic crystals, and compare the field spectra obtained by the Padé approximation and the FFT method.

2 Comparison with FFT method

The basic formula of the Padé approximation with Baker's algorithm is already introduced in Ref. [12]. We present the program of the Padé approximation in Mathlab in the appendix and give a numerical comparison with the FFT method. After obtaining field spectrum $U(f)$ from the time variation output, we use a Lorentzian line-shape function to fit the intensity spectrum $|U(f)|^2$ and calculate mode frequencies and quality factors from the central frequency and the full width of the half-maximum (FWHM) Δf_{FWHM} of each peak by

$$\begin{aligned} f_{\mathrm{mode}} &= f_{\mathrm{center}} \\ Q &= f_{\mathrm{center}}/\Delta f_{\mathrm{FWHM}} \end{aligned} \tag{1}$$

We consider a simple-pole model composed of two poles with the resonant frequencies of 160THz and 162THz and the quality factors of 5000 and 500, respectively. The time sequence of the field component is recorded at a time step of 4.7173×10^{-17} s. Figure 1 shows the intensity spectra obtained by Padé approximation and FFT under different time sequences of field. The results show that the stable intensity spectrum can be obtained from a 2^8 item sequence, and that the intensity spectrum obtained by the FFT method from a 2^{14} item sequence cannot distinguish two peaks. The intensity spectra obtained by the FFT method approachs that of the Padé approximation as the output sequence is 2^{19}- and 2^{20}- item. In Table 1, we compare the mode frequency and quality factor obtained by Padé approximation and FFT for the pole with f = 160THz and Q = 5000. The results show that the mode quality factor obtained by the Padé approximation from a 2^8-item sequence is more exact than that obtained by FFT method from a 2^{20}-item sequence.

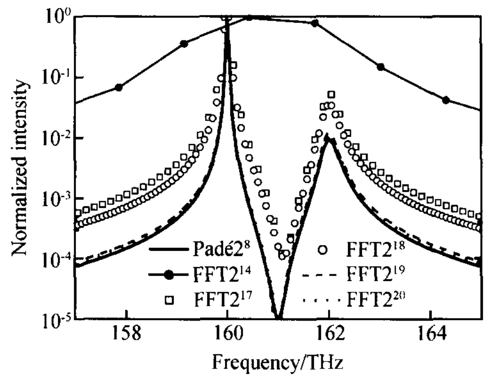

Fig. 1 Frequency spectra obtained by Padé approximation and FFT for two poles under different length of time sequence

Table 1 Frequencies and Q-factors obtained by Padé approximation and FFT method

	Padé	FFT			
Item	2^8	2^{17}	2^{18}	2^{19}	2^{20}
f/ THz	160.00	159.99	160.00	160.00	160.00
Q	5000	2390	3560	4860	4950

3 Photonic band of hexagonal photonic crystals

In this section, we first present the numerical results of the photonic band diagram obtained by the FDTD technique and Padé approximation for the TE-like modes in a hexagonal photonic crystal slab. The top view of the photonic crystal slab is shown in Fig. 2(a). It is formed by a dielectric slab of refractive index 3.4 suspended in air with hexagonal circular air hole arrays. The period of the photonic crystal is a = 500nm, the air hole radius is r = 0.25a, and the slab thickness is 0.5a, all the same as the photonic crystal slab analyzed in Ref. [5]. In our FDTD simulation, the space step Δs is 0.04a and the time step $\Delta t = \Delta s/(3^{1/2} c)$. An initial distribution of the magnetic field components is set to excite different modes. Because the TE-like modes have even symmetry with respect to the central plane of the photonic crystal slab centered at $z = 0$, we only need to perform the FDTD simulation in the upper half space ($z \geq 0$) of a unit cell and impose an even-symmetry condition on the electric field components at the central plane. To deal with the infinite extent of the air region, we impose the first order Mur's absorbing boundary condition[1] at the $z = 5/4a$ plane. Modes at wave vectors in the Γ-K and Γ-M directions have even or odd symmetry with respect to the y and x directions, respectively; thus we add the corresponding symmetry conditions to the electric field components at the $y = 0$ or $x = 0$ plane in order to excite the even and odd modes individually. Furthermore, we find that various modes can be well excited in such a reduced cell with an arbitrary initial field distribution. For boundaries apart from those symmetry planes, the periodic boundary condition is imposed on the electric field components. We perform the FDTD simulation for each wave vector in the Γ-K and Γ-M directions in the two dimensional Brillouin zone, as shown in Fig. 2(b), and then obtain the mode frequencies and quality factors from the FDTD output by the Padé approximation. In Ref. [5], the quality factors are calculated by exciting a single eigenmode by a dipole moment oscillating at its eigenfrequency located in the photonic crystal and observing its decay after switching off the oscillation, after obtaining the photonic band structure by the FFT method from the FDTD output. However, it is difficult to perform single frequency excitation in the FDTD simulation for a cavity with nearly degenerate modes. In the nearly degenerate case, the Padé approximation with Baker's algorithm can still yield a very good field spectrum. For example, we got clear spectra for two nearly degenerate modes with a frequency difference of 0.014% very well in Ref. [4].

In Fig. 3, we plot the intensity spectra of odd modes at $0.1k_K$, where k_K is the wave vector at the K point of the photonic band diagram. The spectra

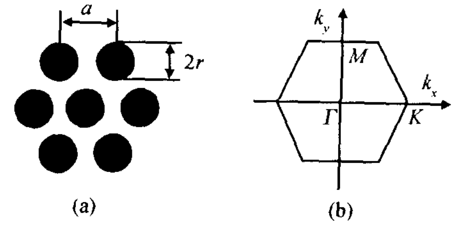

Fig. 2　(a) Top view of the hexagonal photonic crystal; (b) The first Brillouin zone of the hexagonal crystal

obtained by the Padé approximation from the 2^{11}-item and 2^{12}-item FDTD outputs are plotted as the thick solid line and the circles, respectively, which are agreement very well. The intensity spectra obtained by the FFT method from the 2^{14}-, 2^{15}-, and 2^{16}-item FDTD outputs are also plotted in Fig. 3 as the dashed-dotted, the dashed, and the solid lines, where a series of zero is added to FDTD output to calculate the spectra with high resolution. The intensity spectra obtained by the FFT method with a 32 times FDTD output is still much wider than that obtained by the Padé approximation. To obtain quality factors from the intensity spectra obtained by the FFT method is almost impossible because it requires a very long FDTD output series. The quality factors of the two modes obtained by Lorentzian fitting are 670 and 14000, respectively. Based on

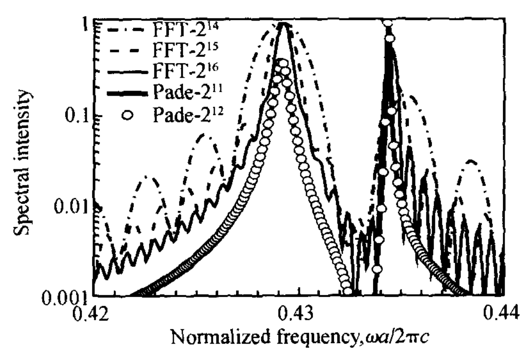

Fig. 3　Spectral intensity of the odd modes at $k = 0.1k_K$ point of the photonic band diagram of the hexagonal photonic crystal slab　2^{11} and 2^{12} steps FDTD outputs are used in the Padé approximation, whereas 2^{14} to 2^{16} steps FDTD outputs are used in the FFT method.

the mode frequencies at each wave vector, we plot the photonic dispersion in the Γ-K and Γ-M directions in Fig. 4, which are obtained by the Padé approximation method from the 2^{11}-item FDTD outputs.

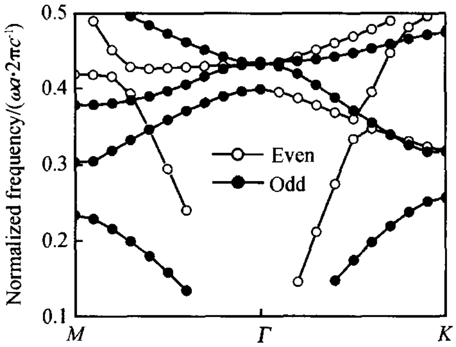

Fig. 4 Photonic band diagram obtained by the Padé approximation from 2^{11}-item FDTD outputs for the hexagonal photonic crystal slab

4 Photonic crystal microcavity

Finally, we consider a microcavity in a two dimensional photonic crystal (PC) with air holes arrayed in a triangular lattice. The dielectric constant is set at $\varepsilon = 11$ and the radius of the air hole $r = 0.32a$, where a is the lattice constant. The photonic crystal structure has a photonic band gap for TE modes between the frequencies $f = 0.221c/a$ to $f = 0.305c/a$. We fill an air hole to form a photonic crystal microcavity. Using a narrow Gaussian pulse $J_z = \exp[-(\frac{t - t_0}{t_w})^2]\cos 2\pi f_0 t$ with $t_w = 3 \times 10^3 dt$, $t_0 = 6 \times 10^3 dt$ where dt is the time step of FDTD simulation, we excite a single guided mode at $f = 0.252c/a$ and show the field distribution in the inset of Fig. 5, we can see the mode is a dipole resonant mode. In Fig. 6, we plot the value of the Q-factor of this mode versus the number N of the PC layers. We can see that the Q-factor exponentially increases with N and the quality factor is large as 8700 when $N = 6$.

5 Conclusion

The FDTD technique combined with the Padé approximation is used to analyze the mode frequencies and quality factors for photonic crystal structures and corresponding microcavities. For the photonic crystals, the field spectrum obtained by the Padé approximation from a 2^{11}-item FDTD output is more accurate than that obtained by the FFT method from a 2^{16}-item FDTD output, especially in the photonic crystal slab case.

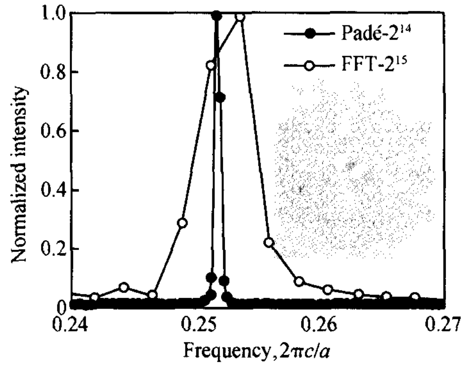

Fig. 5 Spectral intensity of defect mode at $f = 0.252c/a$ obtained from 2^{14}- and 2^{15}-item FDTD outputs by the Padé approximation and the FFT method, respectively, in the two-dimensional triangular photonic crystal microcavity The mode field distribution is shown in the inset, which is a dipole resonant mode.

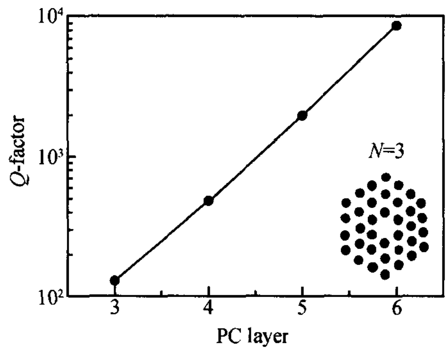

Fig. 6 Mode quality factor versus the number of PC layers for the dipole resonant mode

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Appendix Program of Padé approximation

```
function spec = Pade(data ,dt, f)
 %Pade Calculate the intensity spectrum of a time-domain signal.
 %spec = Pade(data ,dt ,fre)
 %data ,the time-domain signal vector.
 %dt ,the time step.
 %f ,the frequency vector with unit GHz.
 %Author :Wei-Hua Guo ,May 2 ,2004.
fre = f *1.0e9 ; %Hz
hsf = 1/ dt/ 2 ; %Half of the sample frequency
temp = 0.8 *hsf/ max(fre) ;
deciRate = fix(log(temp) / log(2.0)) ;
 %Resample the signal.
for di = 1 :deciRate
    data = decimate(data ,2) ;
end
[siz1 ,siz2] = size(data) ;
if siz1 = = 1
   N = siz2 ;
   if mod(N ,2) = = 0
      N = N - 1 ;
   end
   u = data(1 : N) . ';
elseif siz2 = = 1
   N = siz1 ;
   if mod(N ,2) = = 0
      N = N - 1 ;
   end
   u = data(1 :N) ;
end
tv = (0 : N - 1) . ';
spec = zeros(size(fre)) ;
num = max(size(fre)) ;
for di = 1 :num
    %Prepare Cn
    Cn = u. *exp(-i *2 *pi *fre(di) *(2^deciRate *dt) *
    tv) ;
    %Calculate the spectrum
    spec(di) = fastPade(Cn) ;
end
 %Calculate the intensity spectrum
spec = abs(spec.^2) ;
 %Normalize the intensity spectrum
spec = spec/ max(spec) ;
 %Plot the intensity spectrum
figure ;plot(f ,spec) ;
xlabel('Frequency (GHz)') ;
ylabel('Intensity (a.u.)') ;
 %----------function fastPade------------
function y = fastPade(C)
N = size(C ,1) ;
cYita0 = zeros(N ,1) ;
cYita1 = zeros(N ,1) ;
cZyita1 = zeros(N ,1) ;
cYita0 = C;
cYita1 = [C(1 : N - 1) ;0] ;
cZyita1(2 : N) = cYita1(1 : N - 1) ;
cita0 = 1 ;
```

```
cita1 = 1 ;
for j = 1 :(N - 1)/ 2
    cita0 = cita0-cYita0(N - j + 1)/cYita1(N - j) *cita1;
    cYita0 = cYita0-cYita0(N - j + 1)/cYita1(N - j) *cZyita1;
    cita1 = (cYita0(N - j) *cita1-cYita1(N - j) *cita0)/
        (cYita0(N - j) - cYita1(N - j));
    cYita1 = (cYita0(N - j) *cYita1 - cYita1(N - j) *
        cYita0)/(cYita0(N - j) - cYita1(N - j));
    cZyita1(2:N) = cYita1(1:N - 1);
end
y = sum(cYita0)/cita0;
```

Padé近似在光子晶体模拟中的应用*

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摘要：为了节省时域有限差分(FDTD)法的计算时间,提出了许多将FDTD的时域结果转换到频域的方法.文中介绍了一种基于Baker算法的Padé近似,并展示了其在光子晶体模拟中的应用.对频率为160THz,品质因子为5000的简单谐振子,结果显示Padé近似用2^8时间步数据得到的强度谱比快速傅里叶变换用2^{20}时间步数据得到的强度谱更精确.采用这一Padé近似,光子晶体平板结构中不同波矢对应的模式频率和品质因子及其能带结构可以在很短的FDTD输出结果下得出.另外,Padé近似也用于计算光子晶体微腔的模式频率和品质因子.

关键词：光波导；光子禁带；光子晶体；微腔；有限时域差分法

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