

# Study on the convergence of plane wave expansion method in calculation the band structure of one-dimensional typical phononic crystal

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We study the convergence of plane wave expansion method (PWEM) while calculating the band structure of one-dimensional typical phononic crystals by taking the example of Euler-Bernoulli beam. The both algebraic formats of the conventional and improved PWEM (CPWEM and IPWEM) were derived from the dynamic differential equation. The convergence of the PWEM was analyzed through the low and high eigen-frequencies of highly symmetric points. The numerical experiment shows that the IPWEM has better convergence, which is very efficient to calculate the band structure of one-dimensional typical phononic crystal systems of large elastic mismatch in searching for large band gaps.

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## 1. Introduction

In recent years, phononic crystals (PCs) have received much attention which becomes a hot topic in mechanics, physics and material science [1, 2]. PC is an inspiration drawn from photonic crystals that made of different materials with periodic structure [3, 4]. Propagation of elastic waves in PCs with spatially modulated acoustic impedance is analogous to the behavior of light or electromagnetic waves in photonic crystals [5-7]. Owing to the particular band gap characteristics, PCs can be used to control the propagation of acoustic or elastic waves, and numerous potential engineering applications of the PCs can be appreciated, e.g., vibration isolation, soundproofing and noise reduction and acoustic functional devices (filter, waveguide and diode) [8, 9].

The properties of frequency band gaps in periodic materials have been studied intensively in theoretical predictions and experiments [2, 10]. On the theoretical side, plane wave expansion method (PWEM) [3, 4, 11, 12], transfer matrix method (TMM) [13], and finite difference time domain method (FDTD) [14] are the most popular methods.

Due to the simplicities of theoretical assumptions and the distinct physical meanings, PWEM is widely adopted to calculate the band structures of PCs and predict their band gaps. According to the conventional PWEM (CPWEM), periodic material parameters are expanded in Fourier series based on its lattice structure, and the governing dynamic differential equations are transformed to algebraic eigen-value equations system, by combining Bloch theorem. The band structure will be presented if the eigen-value system is solved in the case of that wave vector changes.

Previous researches show that large contrast in physical properties of constituents is a key factor of large acoustic band gaps [2-4, 15], many researches have focused on designing PC materials for large band gaps [14-16]. The CPWEM works well in most of the studies, but it shows poor convergences on dealing with the system of large elastic mismatch because the Gibbs phenomenon becomes obvious at the material interface where the Fourier series do not converge uniformly [17].

In this paper, we presented the improved PWEM (IPWEM) to calculate the band structure of one-dimensional typical PCs based on CPWEM and Laurent's inverse rule. The theoretical model is built by the combination of dynamic differential equation, Bloch theorem, and Fourier expansion. The advantages of convergence of the IPWEM over the CPWEM are verified through the interpretations of numerical experiment using a PC Euler-Bernoulli beam consisting of aluminum and epoxy.

## 2. Conventional and improving plane wave expansion method

According to the dimensions of their periodicity, PCs can be classified as one-, two-, and three-dimensional (1D, 2D and 3D) PCs, and the aperiodic direction of the general 1D and 2D PCs is assumed infinite. However, some kinds of structures in engineering, e.g., beam and plate, don't satisfy the assumption. These structures are called typical PC structures [18]. Fig. 1 shows a PC Euler-Bernoulli beam consisting  $n$  different kinds beams with periodic constant  $a$ , which is a 1D typical PC structure.

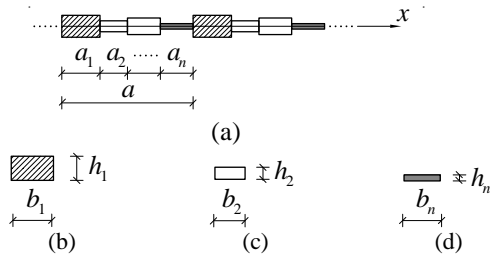


Fig. 1. PC Euler-Bernoulli beam with periodic material and geometric parameters: (a) PC Euler-Bernoulli beam with lattice constant  $a$ , (b) section of beam 1, (c) section of beam 2, (d) section of beam  $n$ .

The differential equation governing the flexural vibration of heterogeneous Euler-Bernoulli beam can be expressed as [19]

$$-\alpha \frac{\partial^2 w}{\partial t^2} = \frac{\partial^2}{\partial x^2} \left[ \beta \frac{\partial^2 w}{\partial x^2} \right] \quad (1)$$

where  $w$  is the transverse displacement.  $\alpha = \rho S$  in which  $\rho$  is the mass density, and  $S$  is the sectional area.  $\beta = EI$  is the flexural rigidity where  $E$  is the Young's modulus and  $I$  is the second moment of inertia. Both of  $\alpha$  and  $\beta$  are periodic functions of position variable  $x$ , so the general form can be given as  $m(x)$ .

Because of the periodicity of PC Euler-Bernoulli beam, the transverse displacement field, according to Bloch theorem, can be expressed as

$$y(x, t) = \exp[i(kx - \omega t)] w_k(x) \quad (2)$$

where  $k$  is the 1D wave vector limited in the first Brillouin zone, which is shown in Fig. 1.  $\Gamma$  and  $X$  are highly symmetric points.  $\omega$  is the circular frequency, and  $w_k(x)$  is the periodic function with the same spatial periodicity of  $m(x)$  and can be expanded in Fourier series as

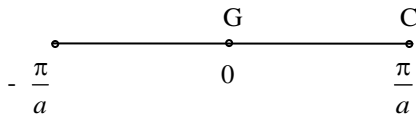


Fig. 2. The first Brillouin zone of 1D lattice.

$$w_k(r) = \sum_{G_1} \exp(iG_1 x) W_{G_1} \quad (3)$$

where  $G_1$  is the 1D reciprocal lattice and  $W_{G_1}$  is the corresponding Fourier coefficient.

$m(x)$  can be also expanded in Fourier series as

$$m(x) = \sum_{G_2} \exp(iG_2 x) M_{G_2} \quad (4)$$

where  $M_{G_2}$  is the corresponding Fourier coefficient of 1D reciprocal lattice  $G_2$ .

We have the following eigenvalue equation by substituting Eqs. (2)-(4) into Eq. (1),

$$\omega^2 \sum_{G_1} \alpha_{G_3 - G_1} W_{G_1} = \sum_{G_1} (k + G_1)^2 (k + G_3)^2 \beta_{G_3 - G_1} W_{G_1} \quad (5)$$

where  $G_3 = G_1 + G_2$ . Eq. (5) is an infinite order eigenvalue problem, so the Fourier series need to be truncated to finite items if we want to solve the equation numerically. Usually, finite reciprocal vectors near the origin are selected. The more reciprocal vectors we choose, the closer the numerical results get to the true value. When  $n$  reciprocal vectors are selected in half axis direction,  $2n+1$  reciprocal vectors are used. We can obtain a matrix equation of  $2n+1$  order from Eq. (5) written in the generalized eigenvalue problem as

$$\omega^2 \mathbf{P} \mathbf{W} = \mathbf{Q} \mathbf{W} \quad (6)$$

where  $\mathbf{P}$  and  $\mathbf{Q}$  are both square matrices of  $2n+1$  order, and  $\mathbf{W}$  is an array of  $2n+1$  order. The entries of  $\mathbf{P}$ ,  $\mathbf{Q}$  and  $\mathbf{W}$  can be expressed as

$$P_{ij} = \alpha_{G_3^{(i)} - G_1^{(j)}} \quad (7)$$

$$Q_{ij} = (k + G_1^{(j)})^2 (k + G_3^{(i)})^2 \beta_{G_3^{(i)} - G_1^{(j)}} \quad (8)$$

$$W_j = W_{G_1^{(j)}} \quad (9)$$

where  $G_1^{(j)}$  and  $G_3^{(i)}$  are the reciprocal vectors in the  $G_1$  and  $G_3$  reciprocal vector spaces with indices  $j$  and  $i$ , respectively.

Wave vectors are picked from the first Brillouin zone which is the interval  $[-\pi/a, \pi/a]$ , and Eq. (6) is solved. We can obtain the relation curve between wave vectors  $k$  and eigen-frequencies  $\omega$ , which is the band structure of PC Euler-Bernoulli beam.

The most serious problem of the CPWEM is the slow convergence at the interface of materials [17]. Based on the theory of Fourier factorizing of product function, Cao et al discovered that it is inappropriate to calculate the Fourier coefficients of a product of two functions using Laurent's rule [11]. Further study shows that the products of elastic parameters function of position and the components of strain tensor are piecewise smooth, bounded, periodic and continuous in 1D PCs, because the products of them are the components of stress tensor. That fits the Laurent's inverse rule [20], so the IPWEM is raised. By the IPWEM,  $1/m(x)$  is expanded in Fourier series and the inverse matrix is adopted. Therefore,  $P_{ij}$  and  $Q_{ij}$  can be rewritten as

$$P_{ij} = [\alpha]_{G_3^{(i)} - G_1^{(j)}}^{-1} \quad (11)$$

$$Q_{ij} = \left(k + G_1^{(j)}\right)^2 \left(k + G_3^{(i)}\right)^2 [\beta]_{G_3^{(i)} - G_1^{(j)}}^{-1} \quad (12)$$

### 3. Numerical experiment and analysis

It is important to note that the IPWEM, by the theory of Fourier factorizing of product function, has the advantage of fast convergence and high precision only if the product functions are continuous. In the case of 1D PCs, there is only one component of stress tensor at the interface, and it is continuous, so the convergence can be well improved and the precision is guaranteed. However, it is noticed that dynamic differential equation of 1D typical PCs is not given in the form of stresses, so the slow convergence may still exist if the IPWEM is applied.

In order to study the convergence of the CPWEM and the IPWEM in calculation the 1D typical PCs, the band structures are calculated while varied numbers of plane wave are chosen ( $n=5,6,\dots,80$ ), and the results are compared to that of the TMM. The TMM is a semi-analytical method, and it can give an implicit expression of corresponding wave vector for any given frequency. We consider the PC Euler-Bernoulli beam consisting of aluminum and epoxy. The material and geometric parameters are listed in Table. 1.

Table. 1 Material and geometric parameters.

	Density $\rho$ ( $\text{kg/m}^3$ )	Young's modulus E (GPa)	Length $l$ (m)	Sectional width $b$ (m)	Sectional height $h$ (m)
Aluminum	2730	77.6	0.05	0.01	0.005
Epoxy	1180	4.35	0.02	0.01	0.01

The first eight bands calculated by the CPWEM, the IPWEM and the TMM are shown in Fig. 3 when  $n=20$ , which is taking abscissa as wave vector  $k$  and ordinate as natural frequency  $f$ . As presented in Fig. 3, the results of the IPWEM agree well with that of the TMM; odd order bands by the CPWEM also agree well with the ones of the TMM and even order bands have a great deviation from the results of the TMM; however, even for the odd order band, the band by the IPWEM is closer to the results by the TMM than the ones by the CPWEM.

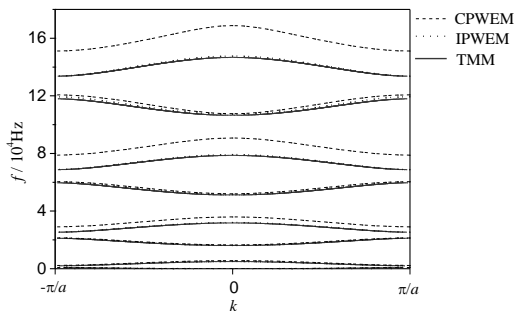
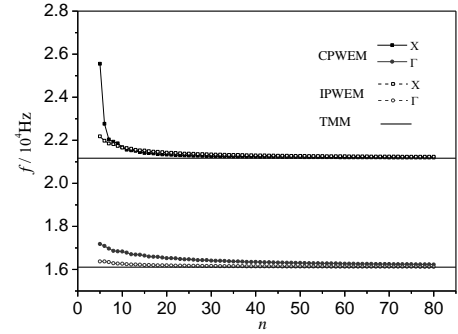
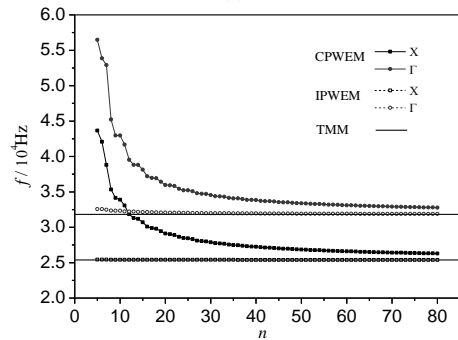


Fig. 3. Band structure of aluminum/epoxy PC Euler-Bernoulli beam by the CPWEM, the IPWEM and the TMM.

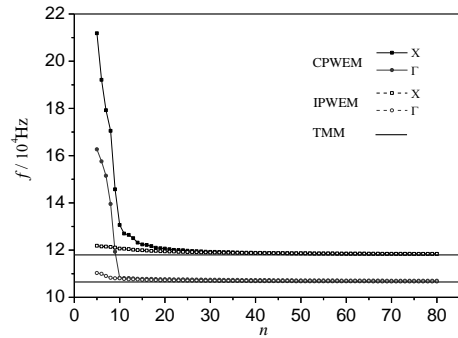
Then we calculate the band structures by the CPWEM, the IPWEM and the TMM, and varied numbers of plane wave are chosen ( $n=5,6,\dots,80$ ). The convergent trends of the fourth and the tenth eigen-frequencies at the highly symmetric points X and  $\Gamma$  are shown in Fig. 4. Being associated with Fig. 3, some conclusions can be drawn from Fig. 4 as follows:



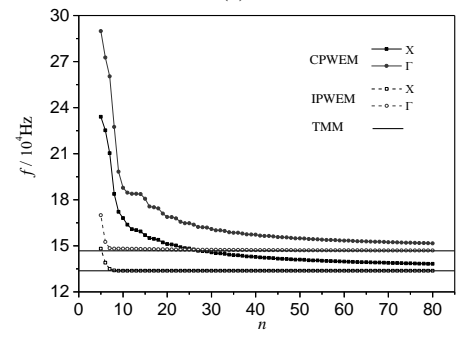
(a)



(b)



(c)



(d)

Fig. 4. The convergent trends of different order eigen-frequencies calculated with varied plane waves of the highly symmetric points: (a) the third order, (b) the fourth order, (c) the seventh order, (d) the eighth order.

**a.** The eigen-frequencies calculated by the CPWEM and the IPWEM always converge to real value downward. It is different from 1D PCs and 2D typical PCs [11, 12]: the frequencies calculated by CPWEM converge to true value downward, while the ones calculated by the IPWEM converge to true value upward.

**b.** The odd and even order eigen-frequencies calculated by the CPWEM show significantly different convergences: the odd order frequencies converge fast even closely to the TMM, while the even order frequencies converge very slowly. However, the convergence of the IPWEM is not sensitive to the orders of frequencies.

**c.** The IPWEM converges faster than the CPWEM either in high or low frequencies, because appropriate formulation of Fourier coefficients of product of two functions is given, which uniformly preserves the continuity of the appropriate across the discontinuities of the elastic parameters function.

Above all, the results show that the IPWEM has good convergence in both high and low frequencies band because the convergence of Fourier series at the interface is effectively improved.

#### 4. Conclusions

In this paper, both algebraic eigenvalue equation systems of the CPWEM and the IPWEM are deduced from dynamic differential equation associated with Bloch theorem and Fourier expansion. The convergences of the CPWEM and the IPWEM in calculating the band structures of typical 1D PCs are studied by taking the example of flexural vibration of PC Euler-Bernoulli beam. The IPWEM shows much better convergence than CPWEM in calculation the band structure of large elastic mismatch 1D typical PCs, because appropriate formulation of Fourier series is given and the at the convergence at the interface of materials is effectively improved. The IPWEM is expected to be widely used to design elastic or acoustic devices and equipments in future researches.

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#### Reference

- [1] Y. Pennec, J. O. Vasseur, B. Djafari-Rouhani, L. Dobrzynski, P. A. Deymier, *Surf. Sci. Rep.* **65**, 229 (2010).
- [2] M. M. Sigalas, M. S. Kushwaha, E. N. Economou, M. Kafesaki, I. E. Psarobas, W. Steurer, *Z. Kristallogr.* **220**, 765 (2005).
- [3] M. S. Kushwaha, P. Halevi, L. Dobrzynski, B. Djafari-Rouhani, *Phys. Rev. Lett.* **71**, 2022 (1993).
- [4] M. S. Kushwaha, P. Halevi, G. Martínez, L. Dobrzynski, B. Djafari-Rouhani, *Phys. Rev. B.*, **49**, 2313 (1994).
- [5] A. Yariv, P. Yeh, *Optical Waves in Crystals*, Wiley, New York (1984).
- [6] J. D. Joannopoulos, S. G. Johnson, J. N. Winn, R. D. Meade, *Photonic Crystals*, Princeton University Press, New Jersey (2008).
- [7] K. B. Thapa, P. C. Pandey, S. Singh, *Optoelectron. Adv. Mater. – Rapid Commun.* **4**, 909 (2010).
- [8] A. Khelif, A. Choujaa, S. Benchabane, B. Djafari-Rouhani, V. Laude, *Appl. Phys. Lett.* **84**, 4400 (2004).
- [9] X. F. Li, X. Ni, L. Feng, M. H. Lu, C. He, Y. F. Chen, *Phys. Rev. Lett.* **106**, 084301 (2011).
- [10] R. Martínez-Sala, J. Sancho, J. V. Sánchez, V. Gómez, J. Linares, F. Meseguer, *Nature.* **378**, 241 (1995).
- [11] Y. J. Cao, Z. L. Hou, Y. Y. Liu, *Phys. Lett. A.* **327**, 247 (2004).
- [12] Y. Zhang, Z. Ni, L. Han, Z. Zhang, H. Chen, *Optoelectron. Adv. Mater. – Rapid Commun.* **5**, 870 (2011).
- [13] M. M. Sigalas, C. M. Soukoulis. *Phys. Rev. B.* **51**, 2780 (1995).
- [14] M. M. Sigalas, N. García, *J. Appl. Phys.* **87**, 3122 (2000).
- [15] Q. N. Liu, *Acta Phys. Sin-ChEd.* **60**, 034301 (2011).
- [16] J. H. Wen, G. Wang, Y. Z. Liu, D. L. Yu, *Acta Phys. Sin-ChEd.* **53**, 3384 (2004).
- [17] L. F. Li, *J. Opt. Soc. Am. A.* **13**, 1870 (1996).
- [18] X. S. Wen, J. H. Wen, D. L. Yu, G. Wang, Y. Z. Liu, X. Y. Han, *Phononic Crystals*, National Defense Industry Press, Beijing (2009).
- [19] R. W. Clough, J. Penzien, *Dynamics of Structures* (3<sup>rd</sup> edition), Computer & Structure Inc., Berkeley (1995).
- [20] A. Zygmund, *Trigonometric Series*, Cambridge University Press, Cambridge (1977).

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