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COMMENT

Comment on "Band gaps structure and semi-Dirac point of two-dimensional function photonic crystals" by Si-Qi Zhang *et al.*[*]

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Recently, Zhang *et al.* (*Chin. Phys. B* **26** 024208 (2017)) investigated the band gap structures and semi-Dirac point of two-dimensional function photonic crystals, and the equations for the plane wave expansion method were induced to obtain the band structures. That report shows the band diagrams with the effects of function coefficient k and medium column r_a under TE and TM waves. The proposed results look correct at first glance, but the authors made some mistakes in their report. Thus, the calculated results in their paper are incorrect. According to our calculations, the errors in their report are corrected, and the correct band structures also are presented in this paper.

Keywords: two-dimensional function photonic crystals, photonic band gaps, plane wave expansion method, Monte Carlo method

PACS: 42.70.Qs, 78.20.Bh, 73.20.At **DOI:** 10.1088/1674-1056/27/1/014205

1. Introduction

Recently, Zhang *et al.*[1] studied the band gap structures and semi-Dirac point of two-dimensional (2D) function photonic crystals (FPCs) by the plane wave expansion (PWE) method. The configuration of the 2D FPCs is the square lattice, which is filled with the dielectric cylinders in the air background. The dielectric constant of the inserted dielectric cylinders is a function of space coordinate r, which can be expressed as $\varepsilon(r) = k \cdot r + 9$, where k is named the function coefficient, and $0 \leq r \leq r_a$, with r_a being the radius of the inserted dielectric cylinder. In their report, the calculation formulas of the PWE method are also induced to obtain the band diagrams of the 2D FPCs. Obviously, equation (17) in their paper is the key to compute the dispersion relations of the 2D FPCs, which can be written as[1]

$$\varepsilon^{-1}(\boldsymbol{G}_{||}) = \begin{cases} \dfrac{1}{\varepsilon_b}(1-f) + \dfrac{2f}{r_a^2}\int_0^{r_a} r \dfrac{1}{\varepsilon_a(r)}\,\mathrm{d}r, & (\boldsymbol{G}_{||} = 0), \\ \dfrac{2f}{r_a^2}\int_0^{r_a} r \dfrac{1}{\varepsilon_a(r)} J_0(\boldsymbol{G}_{||}\cdot r)\,\mathrm{d}r - \dfrac{2f}{\varepsilon_b}\dfrac{J_1(\boldsymbol{G}_{||}\cdot r_a)}{\boldsymbol{G}_{||}\cdot r_a}, & (\boldsymbol{G}_{||} \neq 0), \end{cases} \tag{1}$$

where $\boldsymbol{G}_{||}$ is the reciprocal vector. In Ref. [1], the Fourier transform of the dielectric constant for the 2D FPCs is calculated by Eq. (1). Figures 2–8 in the report of Zhang *et al.* can be directly computed by Eqs. (17), (19), and (20) in Ref. [1] under TM and TE waves. Those results look correct at first glance. However, there are some mistakes which were ignored by Zhang *et al*. In their report, they considered some special cases, such as $r_a = 0.65a$ and $r_a = 0.8a$. Obviously, in those cases, equation (1) is unsuitable for the calculation of the Fourier transform of the dielectric constant for the 2D FPCs since some part of the inserted dielectric cylinders will overlap with each other. Equation (1) cannot describe such a situation well. Thus, we have to find a new way to solve this problem. Recently, Zhang *et al.* proposed some new approaches to modify the PWE method with a meshed grid technique[2] or based on the Monte Carlo method[3] to calculate the band structures of 2D photonic crystals (PCs) which possess arbitrary-shaped filler and any lattice. As we know, computing $\varepsilon^{-1}(\boldsymbol{G}_{||})$ is the key to obtain the band structures of 2D PCs. Therein, the value of $\varepsilon^{-1}(\boldsymbol{G}_{||})$ can also be obtained by the numeral calculations. The details of the modified PWE methods can be found in Refs. [2] and [3]. In this paper, the PWE method based on the Monte Carlo method will be used to calculate the band diagrams as mentioned in Ref. [1], and correct the errors in Ref. [1]. The equations of calculations can be found in Ref. [3].

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2. Numerical results and analysis

Firstly, a numerical example is used to show that equation (1) cannot be utilized to compute the Fourier transform of the 2D PCs directly when the inserted dielectric cylinders overlap with each other. In Fig. 1, the topology and unit cell of the 2D PCs with square lattices are plotted. As shown in Fig. 1(a), in the numerical example, the homogeneous and isotropic air cylinders are inserted in the dielectric background with square lattices to construct the 2D PCs. The radius of the inserted air cylinders and the lattice constant are considered as R and a, respectively. We also assume that the relative permittivity of the dielectric background is ε_{d}. The initial parameters are $\varepsilon_{\mathrm{d}} = 13$ and $R = 0.55a$, respectively. We can see from Fig. 1(b) that if $R = 0.55a$, the inserted air rods will overlap with each other (see the shaded parts of Fig. 1(b)). In order to verify the correctness of the modified PWE method based on the Monte Carlo method, the finite-difference frequency-domain (FDFD) method[4] is also used to calculate the band structures of such 2D PCs under TE wave as mentioned in Ref. [1], and makes a comparison with the proposed PWE method. In order to ensure that the calculations have sufficient accuracy, for the PWE method, 1225 plane waves and 120000 random sampling points are used in the Monte Carlo method. For the FDFD method, the unit cell of the 2D PCs is divided into 130×130 grids. The calculated dispersion curves of the 2D PCs with square lattices by the different methods are displayed in Fig. 2. As shown in Fig. 2(a), the red open circles (the FDFD method) match quite well with the blue solid lines (the modified PWE method based on the Monte Carlo method). From the results in Fig. 2(a), we know that the modified PWE method based on the Monte Carlo method can be used to obtain the band structures of the 2D PCs in such a case ($R = 0.55a$), and also has sufficient accuracy. It can also be seen from Fig. 2(b) that the band diagram obtained by the approach in Ref. [1] is totally different from that present in Fig. 2(a). Comparing Fig. 2(a) to Fig. 2(b), we can find that the equations in Ref. [1] are unsuitable to calculate the band structures of the 2D PCs in such a case ($R = 0.55a$). As mentioned above, mistakes have been made by Zhang *et al.* in Ref. [1], and the corrected results will be presented in the following.

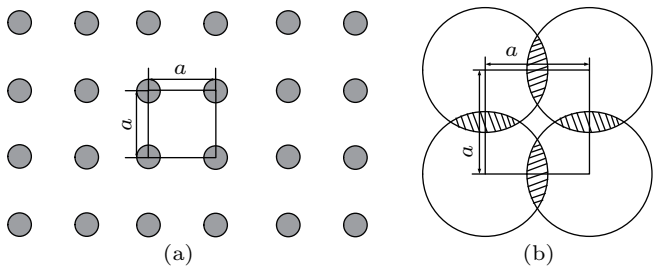


Fig. 1. (a) Topology and (b) unit cell of the 2D PCs with square lattices.

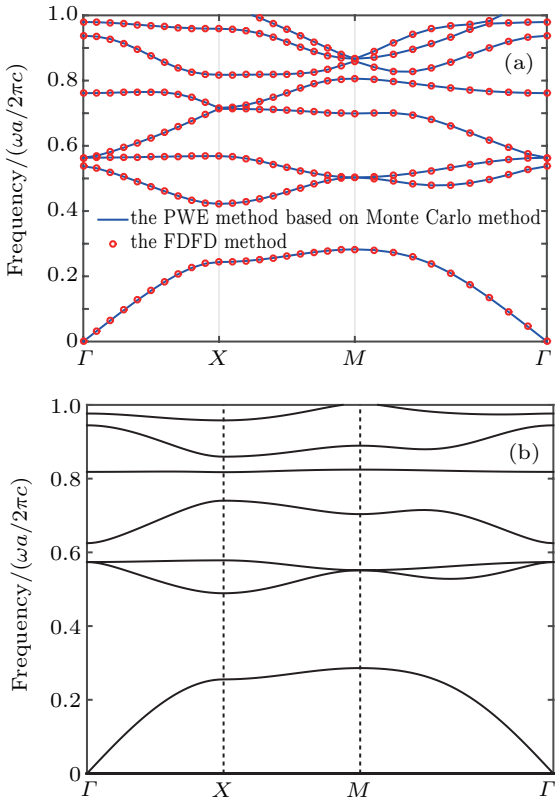


Fig. 2. (color online) The calculated dispersion curves of the 2D PCs with square lattices by different methods: (a) the PWE method based on Monte Carlo method and FDFD method, (b) the approach in Ref. [1].

We can re-calculate the band structures of the 2D FPCs in Ref. [1]. In Fig. 3, the band structures of 2D conventional PCs with the triangle lattices are plotted under TE and TM waves (Fig. 2 in Ref. [1]), where $\varepsilon_{\mathrm{b}} = 1$, $\varepsilon_{\mathrm{a}} = 9$, and $r_{\mathrm{a}} = 0.65a$. The red region represents the band gaps. We can see from Fig. 3 that the results in Fig. 2 of Ref. [1] are not correct. There is only one band gap under the TE wave, and there is no band gap under the TM wave. Similarly, figures 4–7 are also plotted to make comparisons with Figs. 3–6 in Ref. [1], where the same situations and parameters of the 2D FPCs are considered. As shown in Figs. 4–7, most of the results in Figs. 3–6 of Ref. [1] are not corrected except for Figs. 3(a) and 4(a) in Ref. [1]. In Figs. 4–7, if $k = 1.8 \times 10^6$, the band structures of the 2D FPCs can be tuned by changing r_{a} under TE and TM waves. If $r_{\mathrm{a}} = 0.26a$ (see Fig. 4), two wider band gaps can be observed under TE wave but no band gaps can be obtained under TM wave. Such results are totally different from those shown in Fig. 3(b) of Ref. [1]. If $r_{\mathrm{a}} = 0.3a$ (see Fig. 5), three band gaps can be obtained under TE wave while a narrow band gap can be seen near the frequency of 0.5 under TM wave. If $r_{\mathrm{a}} = 0.65a$ (see Fig. 6), there do not exist any band gaps under TE and TM waves. The results do not totally agree with Fig. 5 in Ref. [1]. If $r_{\mathrm{a}} = 0.8a$ (see Fig. 7), there is only one band gap under TE wave but two band gaps were shown in Ref. [1], and the band gaps also cannot be found under TM wave. Obviously, figures 3–6 in Ref. [1] are incorrect except for Figs. 3(a) and 4(a). Although the number and locations

of band gaps in the 2D FPCs can be tuned by changing r_a, the trends of the band gaps are quite different from the results proposed by Zhang *et al.*, and only narrow band gaps can be obtained under TE wave when $r_a = 0.65a$ or $r_a = 0.8a$.

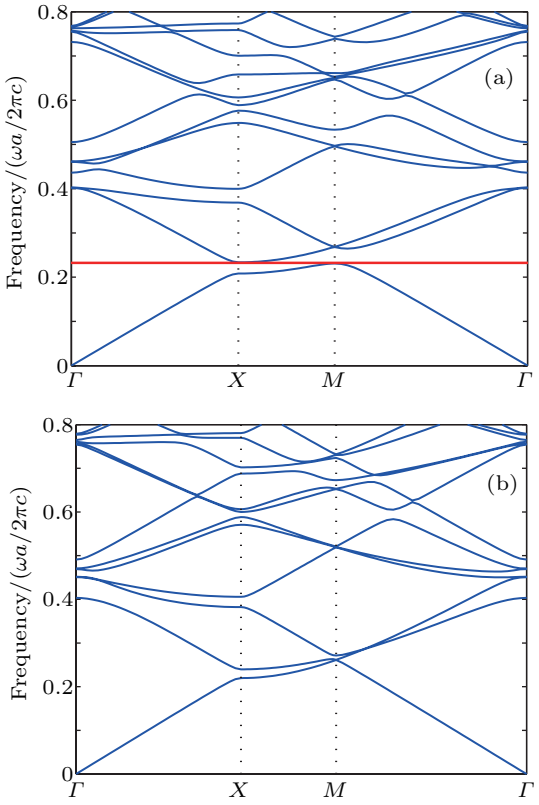


Fig. 3. (color online) The band structures of 2D conventional PCs with the triangle lattices, where $\varepsilon_b = 1$, $\varepsilon_a = 9$, and $r_a = 0.65a$. (a) TE wave, (b) TM wave.

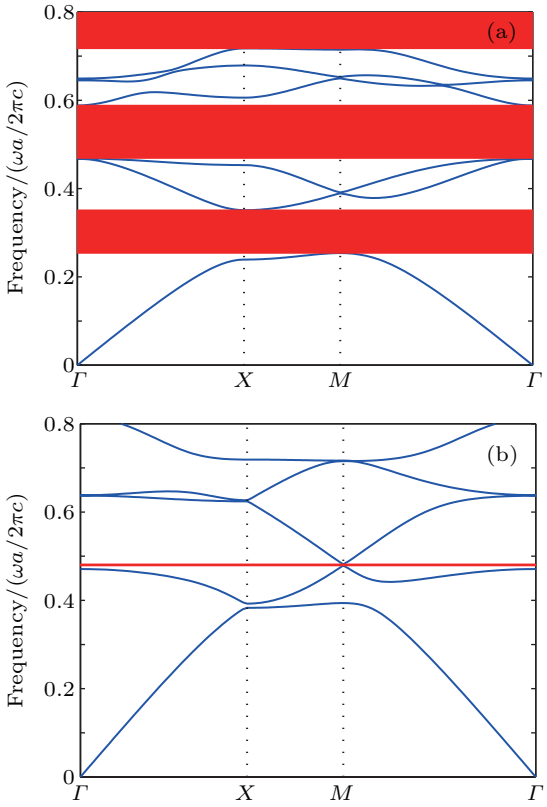


Fig. 5. (color online) The band structures of 2D FPCs with the triangle lattices, where $\varepsilon_b = 1$, $\varepsilon_a = kr+9$, $k = 1.8\times10^6$, and $r_a = 0.3a$. (a) TE wave, (b) TM wave.

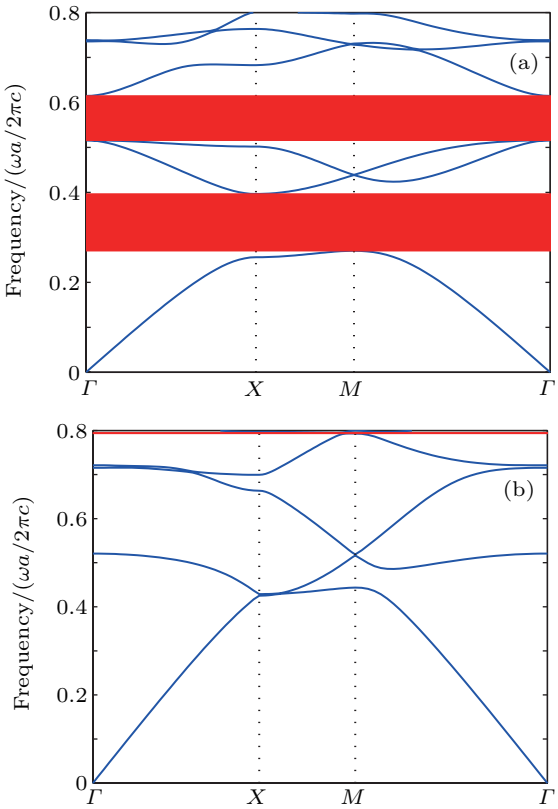


Fig. 4. (color online) The band structures of 2D FPCs with the triangle lattices, where $\varepsilon_b = 1$, $\varepsilon_a = kr+9$, $k = 1.8\times10^6$, and $r_a = 0.26a$. (a) TE wave, (b) TM wave.

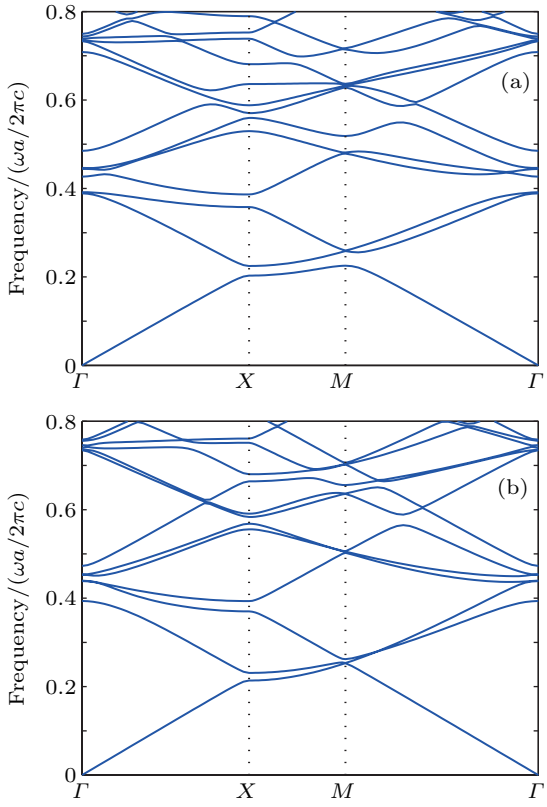


Fig. 6. (color online) The band structures of 2D FPCs with the triangle lattices, where $\varepsilon_b = 1$, $\varepsilon_a = kr+9$, $k = 1.8\times10^6$, and $r_a = 0.65a$. (a) TE wave, (b) TM wave.

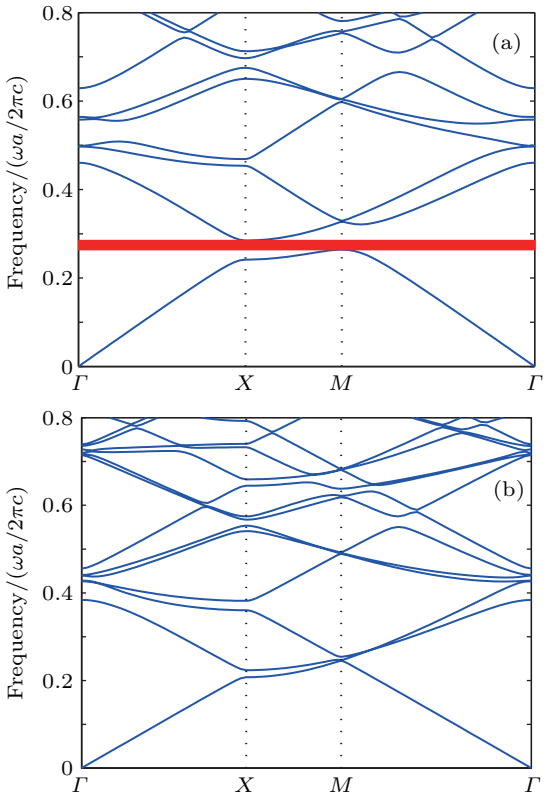


Fig. 7. (color online) The band structures of 2D FPCs with the triangle lattices, where $\varepsilon_b = 1$, $\varepsilon_a = kr + 9$, $k = 1.8 \times 10^6$, and $r_a = 0.8a$. (a) TE wave, (b) TM wave.

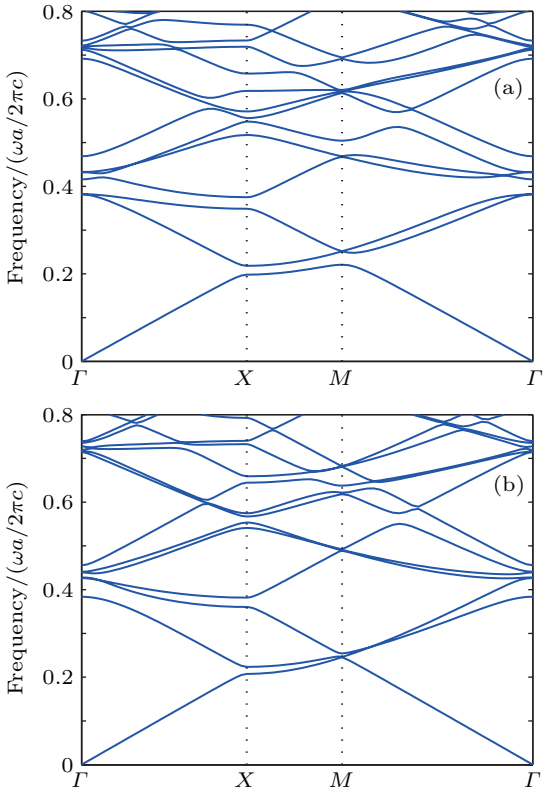


Fig. 8. (color online) The band structures of 2D FPCs with the triangle lattices, where $\varepsilon_b = 1$, $\varepsilon_a = kr + 9$, $k = 3.6 \times 10^6$, and $r_a = 0.65a$. (a) TE wave, (b) TM wave.

It is noticed that one semi-Dirac point can also be found in the case of $r_a = 0.3a$ (Fig. 5), which is near the frequency of 0.6. In Figs. 8 and 9, the function coefficient k effect on the band structures of the 2D FPCs is also given, which are used to make comparison with Figs. 7 and 8 in Ref. [1]. As shown in Fig. 8, if $k = 3.6 \times 10^6$ and $r_a = 0.65a$, there is no band gap in the band diagrams under TM and TE waves. It can be seen from Fig. 9 that if $k = -1.8 \times 10^6$ and $r_a = 0.65a$, only one band gap can be obtained under TE wave, and there are no band gaps under TM wave. Comparing Fig. 8 with Fig. 7 in Ref. [1], we can see that the dispersion curves of the 2D FPCs in the two figures are completely different, and figure 7 in Ref. [1] is incorrect. According to the results in Fig. 8, we can see that the semi-Dirac points do not exist. Similarly, the different trends of the band structures can also be observed between Fig. 9 and Fig. 8 in Ref. [1]. As shown in Fig. 9(a), one band gap can be obtained under TE wave, and there is no band gap under TM wave. The semi-Dirac points cannot be found in Fig. 9.

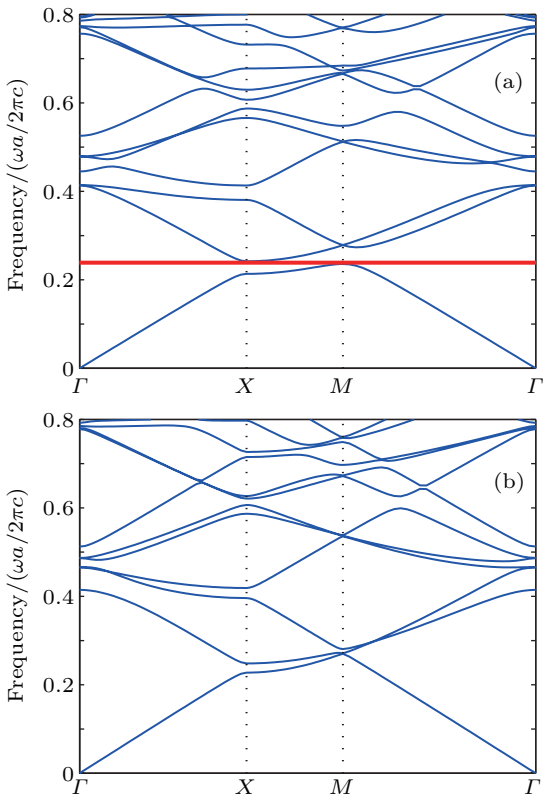


Fig. 9. (color online) The band structures of 2D FPCs with the triangle lattices, where $\varepsilon_b = 1$, $\varepsilon_a = kr + 9$, $k = -1.8 \times 10^6$, and $r_a = 0.65a$. (a) TE wave, (b) TM wave.

3. Conclusion and perspectives

In summary, the modified PWE method based on the Monte Carlo method is used to obtain the band structures of the 2D FPCs in Ref. [1]. For the case of $r_a > 0.5a$, equation (1) (analytical solution) is unsuitable to be used to calculate directly the Fourier transform of the dielectric constant for the

2D FPCs to obtain the band structures. The results obtained by Zhang *et al.* are incorrect. In this paper, the corrected results are presented. We also point out that the modified PWE method is a better way to compute the band diagrams of 2D FPCs when $r_a > 0.5a$.

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