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# A new wave theory of photonic crystals

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#### A new wave theory of photonic crystals

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In this paper, we have presented a wave theory method to study 1D photonic crystals (PCs), and give the new transfer matrix, dispersion relation, and transmissivity. We have calculated the dispersion relation and transmissivity with the new wave theory and the transfer matrix method, and find the dispersion relation and transmissivity are identical for the two kinds of methods. The new wave method can be also used to study 2D and 3D PCs.

Keywords: photonic crystals; transmissivity; dispersion relation

#### 1. Introduction

Photonic crystals (PCs) are artificial materials with periodic variations in refractive index, which control photons in a way comparable to the way semiconductors control electrons, and have inspired extensive study since their emergence in the late 1980s [1,2]. PCs are designed to affect the propagation of light [3–6]. An important feature of the PCs is that there are allowed and forbidden ranges of frequencies at which light propagates in the direction of index periodicity. Due to the forbidden frequency range, known as photonic band gap [7,8], which prevents light from propagating in certain directions at specific frequencies, it is analogous to the electron band gap in semiconductors.

Thus, numerous applications of PCs have been proposed in improving the performance of optoelectronic and microwave devices such as high-efficiency semiconductor lasers, right emitting diodes, wave guides, optical filters, high-Q resonators, antennas, frequency-selective surface, optical wave guides and sharp bends [9], WDM-devices [10,11], splitters and combiners [12]. optical limiters and amplifiers [13,14].

At present, there are some numerical methods to study PCs, such as: the plane-wave expansion method [15–17], the finite-difference time-domain method [18–21], the transfer matrix method (TMM) [22,23], the finite element method (FE) [24–26], the scattering matrix method [27], the Green's function method [28], and so on. In Refs. [29,30], the authors give the quantum wave equation of a single photon. In Ref. [31], we have given the quantum wave

equations of free and non-free photon. In this paper, we study the 1D PCs by the wave equations of photon [31], and give the new dispersion relation, transmissivity, and reflectivity. By calculation, we find the results are identical to the transfer matrix method [22,23]. The new wave method can be also used to study 2D and 3D PCs.

The paper is organized as follows. In Section 2, the wave equation and probability current density of photon are given. In Section 3, with the wave theory of photon, the transmissivity and reflectivity of 1D PCs are given. In Section 4, we give the dispersion relation and transfer matrix. In Section 5, we give the numerical analysis and compare the results of wave theory of photon with the transfer matrix method. Finally, a summary is given in Section 6.

# 2. The wave equation and probability current density of a photon

The wave equations of a free and non-free photon have been obtained in Ref. [31], they are

$$i\hbar\frac{\partial}{\partial t}\vec{\psi}(\vec{r},t) = c\hbar\nabla \times \vec{\psi}(\vec{r},t), \qquad (1)$$

and

$$i\hbar\frac{\partial}{\partial t}\vec{\psi}(\vec{r},t) = c\hbar\nabla \times \vec{\psi}(\vec{r},t) + V\vec{\psi}(\vec{r},t), \qquad (2)$$

where  $\vec{\psi}(\vec{r}, t)$  is the vector wave function of photon, and V is the potential energy of photon in medium. In the medium of refractive index n, the photon's potential energy V is [31]

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$$V = \hbar\omega(1 - n). \tag{3}$$

The conjugate of Equation (2) is

$$-i\hbar\frac{\partial}{\partial t}\vec{\psi}^*(\vec{r},t) = c\hbar\nabla \times \vec{\psi}^*(\vec{r},t) + V\vec{\psi}^*(\vec{r},t).$$
(4)

Multiplying the Equation (2) by  $\vec{\psi}^*$ , the Equation (4) by  $\vec{\psi}$ , and taking the difference, we get

$$i\hbar\frac{\partial}{\partial t}\left(\vec{\psi}^*\cdot\vec{\psi}\right) = c\hbar\left(\vec{\psi}^*\cdot\nabla\times\vec{\psi} - \vec{\psi}\cdot\nabla\times\vec{\psi}^*\right)$$
$$= c\hbar\nabla\cdot\left(\vec{\psi}\times\vec{\psi}^*\right),\tag{5}$$

i.e.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0, \tag{6}$$

where

$$o = \vec{\psi}^* \cdot \vec{\psi},\tag{7}$$

and

$$J = ic\psi \times \psi^*, \tag{8}$$

are the probability density and probability current density, respectively.

By the method of separation variable

$$\vec{\psi}(\vec{r},t) = \vec{\psi}(\vec{r})f(t), \qquad (9)$$

the time-dependent Equation (2) becomes the time-independent equation

$$c\hbar\nabla \times \vec{\psi}(\vec{r}) + V\vec{\psi}(\vec{r}) = E\vec{\psi}(\vec{r}), \qquad (10)$$

where E is the energy of photon in medium.

By taking curl in (10), when  $\frac{\partial V}{\partial x_i} = 0$ , (i = 1, 2, 3), the Equation (10) becomes

$$(\hbar c)^2 (\nabla (\nabla \cdot \vec{\psi}(\vec{r})) - \nabla^2 \vec{\psi}(\vec{r})) = (E - V)^2 \vec{\psi}(\vec{r}).$$
(11)

Choosing transverse gange

$$\nabla \cdot \vec{\psi}(\vec{r}) = 0, \tag{12}$$

the Equation (11) becomes

$$\nabla^2 \vec{\psi}(\vec{r}) + \left(\frac{E-V}{\hbar c}\right)^2 \vec{\psi}(\vec{r}) = 0.$$
(13)

With Equations (12) and (13), we should study 1D PCs by the wave theory approach.

#### 3. The new wave theory of 1D PCs

For 1D PCs, we should define and calculate its new dispersion relation and transmissivity. The 1D PCs structure is shown in Figure 1.

In Figure 1,  $\psi_I$ ,  $\psi_R$ ,  $\psi_T$  are the wave functions of incident, reflection, and transmission photon, respectively, and they can be written as

$$\vec{\psi}(\vec{r},t) = \vec{\psi}_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)} = \psi_x \vec{i} + \psi_y \vec{j} + \psi_z \vec{k}, \qquad (14)$$

By transverse gange  $\nabla \cdot \vec{\psi}(\vec{r}) = 0$ , we get

$$k_x \psi_x + k_y \psi_y + k_z \psi_z = 0.$$
 (15)



Figure 1. The structure of 1D PCs.

In Figure 1, the photon travels along with the *x*-axis, the wave vector  $k_y = k_z = 0$  and  $k_x \neq 0$ . By Equation (15), we have

$$\psi_x = 0, \tag{16}$$

so the total wave function of the photon is

$$\vec{\psi} = \vec{\psi}_y \vec{j} + \vec{\psi}_z \vec{k},\tag{17}$$

the Equation (13) becomes two component equations

$$\nabla^2 \psi_y + \left(\frac{E-V}{\hbar c}\right)^2 \psi_y = 0, \qquad (18)$$

$$\nabla^2 \psi_z + \left(\frac{E-V}{\hbar c}\right)^2 \psi_z = 0. \tag{19}$$

In Figure 1, the wave functions of incident, reflection, and transmission photon can be written as:

$$\vec{\psi}_{I} = F_{y} e^{i(\vec{k}\cdot\vec{r}-\omega t)}\vec{j} + F_{z} e^{i(\vec{k}\cdot\vec{r}-\omega t)}\vec{k},$$
(20)

$$\vec{\psi}_{R} = F_{v}^{'} e^{i(\vec{k}\cdot\vec{r}-\omega t)}\vec{j} + F_{z}^{'} e^{i(\vec{k}\cdot\vec{r}-\omega t)}\vec{k}, \qquad (21)$$

$$\vec{\psi}_T = D_y e^{i(\vec{k}\cdot\vec{r}-\omega t)}\vec{j} + D_z e^{i(\vec{k}\cdot\vec{r}-\omega t)}\vec{k},\qquad(22)$$

where  $F_y$ ,  $F_z$ ,  $F'_y$ ,  $F'_z$ ,  $D_y$ , and  $D_z$  are their amplitudes. The component form of Equation (1) is

$$\begin{cases}
i\hbar\frac{\partial}{\partial t}\psi_{x} = \hbar c \left(\frac{\partial\psi_{z}}{\partial y} - \frac{\partial\psi_{y}}{\partial z}\right) \\
i\hbar\frac{\partial}{\partial t}\psi_{y} = \hbar c \left(\frac{\partial\psi_{x}}{\partial z} - \frac{\partial\psi_{z}}{\partial x}\right) , \\
i\hbar\frac{\partial}{\partial t}\psi_{z} = \hbar c \left(\frac{\partial\psi_{y}}{\partial x} - \frac{\partial\psi_{x}}{\partial y}\right)
\end{cases}$$
(23)

substituting Equations (14) and (16) into (23), we have

$$\psi_z = i\psi_y, \tag{24}$$

the probability current density becomes

$$J = ic\vec{\psi} \times \vec{\psi}^* = 2c|\psi_z|^2 \vec{i} = 2c|\psi_{0z}|^2 \vec{i}, \qquad (25)$$

where

$$\psi_z = \psi_{0z} e^{i(k \cdot \vec{r} - \omega t)}, \qquad (26)$$

the  $\psi_{0z}$  is  $\psi_z$  amplitude.

For the incident, reflection, and transmission photon, their probability current density  $J_I$ ,  $J_R$ ,  $J_T$  are

$$J_I = 2c |F_z|^2,$$
 (27)

$$J_R = 2c |F_z|^2, (28)$$

$$J_T = 2c |D_z|^2,$$
 (29)

We can define a new wave transmissivity T and reflectivity R as

$$T = \frac{J_T}{J_I} = \left| \frac{D_z}{F_z} \right|^2, \tag{30}$$

$$R = \frac{J_R}{J_I} = \left|\frac{F_z'}{F_z}\right|^2.$$
 (31)

#### 4. A new wave transmissivity and dispersion relation

Since the probability current densities are relevant to the z component amplitudes of wave function, we should only solve the z component equation (19) for the 1D PCs, which is shown in Figure 2.

With Equation (19), the photon's new wave equation in mediums A and B are

$$\frac{\partial^2 \psi_A}{\partial x^2} + k_A^2 \psi_A = 0 \quad (0 < x < a), \tag{32}$$

$$\frac{\partial^2 \psi_B}{\partial x^2} + k_B^2 \psi_B = 0 \quad (a < x < a + b), \tag{33}$$

where

$$k_{A} = \frac{E - V_{a}}{\hbar c} = \frac{E - \hbar \omega (1 - n_{a})}{\hbar c} = \frac{\omega}{c} n_{a} = \frac{2\pi}{\lambda} n_{a},$$
(34)
$$k_{B} = \frac{E - V_{b}}{\hbar c} = \frac{E - \hbar \omega (1 - n_{b})}{\hbar c} = \frac{\omega}{c} n_{b} = \frac{2\pi}{\lambda} n_{b},$$
(35)

where  $\lambda = 2\pi c/\omega$  is the photon wave length in vacuum,  $V_a = \hbar\omega(1-n_a)$  ( $V_b = \hbar\omega(1-n_b)$ ) is the potential energy of the photon in medium A(B), and  $n_a(n_b)$  is refractive index of medium A(B). In order to simplify, the index z is omitted, i.e.  $\psi_{zA}(\psi_{zB})$  is written as  $\psi_A(\psi_B)$ .

The solutions of Equations (32) and (33) are

$$\psi_A = A_1 e^{ik_A x} + A_2 e^{-ik_A x} \quad (0 < x < a), \quad (36)$$

$$\psi_B = B_1 e^{ik_B x} + B_2 e^{-ik_B x} \quad (a < x < a + b).$$
(37)

By Bloch law, there is

$$\begin{aligned} \psi(a+b < x < 2a+b) \\ &= \psi(0 < x < a)e^{ik(a+b)} \\ &= \left(A_1 e^{ik_A(x-(a+b))} + A_2 e^{-ik_A(x-(a+b))}\right)e^{ik(a+b)}, \end{aligned}$$
(38)

where k is Bloch wave vector.



Figure 2. The structure of 1D PCs.

At x = a, by the continuation of wave function and its derivative, we have

$$A_{1}e^{ik_{A}a} + A_{2}e^{-ik_{A}a} = B_{1}e^{ik_{B}a} + B_{2}e^{-ik_{B}a},$$
(39)  
$$ik_{A}A_{1}e^{ik_{A}a} - ik_{A}A_{2}e^{-ik_{A}a} = ik_{B}B_{1}e^{ik_{B}a} - ik_{B}B_{2}e^{-ik_{B}a},$$
(40)

At x = a + b, by the continuation of wave function and its derivative, we have

$$A_1 e^{ik(a+b)} + A_2 e^{ik(a+b)} = B_1 e^{ik_B(a+b)} + B_2 e^{-ik_B(a+b)},$$
(41)

$$ik_A A_1 e^{ik(a+b)} - ik_A A_2 e^{ik(a+b)}$$
  
=  $ik_B B_1 e^{ik_B(a+b)} - ik_B B_2 e^{-ik_B(a+b)}$ , (42)

and we obtain the follows equations set

$$\begin{cases} A_1 e^{ik_A a} + A_2 e^{-ik_A a} = B_1 e^{ik_B a} + B_2 e^{-ik_B a} \\ ik_A A_1 e^{ik_A a} - ik_A A_2 e^{-ik_A a} = ik_B B_1 e^{ik_B a} - ik_B B_2 e^{-ik_B a} \\ A_1 e^{ik(a+b)} + A_2 e^{ik(a+b)} = B_1 e^{ik_B(a+b)} + B_2 e^{-ik_B(a+b)} \\ ik_A A_1 e^{ik(a+b)} - ik_A A_2 e^{ik(a+b)} = ik_B B_1 e^{ik_B(a+b)} \\ - ik_B B_2 e^{-ik_B(a+b)}, \end{cases}$$
(43)

the necessary and sufficient condition of Equation (43) nonzero solution is its coefficient determinant equal to zero

$$\begin{vmatrix} e^{ik_Aa} & e^{-ik_Aa} & -e^{ik_Ba} & -e^{-ik_Ba} \\ k_Ae^{ik_Aa} & -k_Ae^{-ik_Aa} & -k_Be^{ik_Ba} & k_Be^{-ik_Ba} \\ e^{ik(a+b)} & e^{ik(a+b)} & -e^{ik_B(a+b)} & -e^{-ik_B(a+b)} \\ k_Ae^{ik(a+b)} & -k_Ae^{ik(a+b)} & -k_Be^{ik_B(a+b)} & k_Be^{-ik_B(a+b)} \end{vmatrix} = 0,$$
(44)

simplifying Equation (44), we obtain the new wave dispersion relation

$$\cos(k(a+b)) = \cos(k_A a) \cos(k_B b)$$
$$-\frac{1}{2} \left(\frac{1}{k_A} + \frac{1}{k_B}\right) \sin(k_A a) \sin(k_B b).$$
(45)

In the following, we should give the wave function of photon in every medium, and the transmission wave function. In Figure 3, we give the simplification form of wave function in every medium, such as symbols  $A_{k_A}^1$  and  $A_{-k_A}^1$  express simplifying wave function of medium A in the first period, it express wave function

$$\psi_{A^1}(x) = A^1_{k_A} e^{ik_A x} + A^1_{-k_A} e^{-ik_A x}, \qquad (46)$$

in medium *B* of first period, the symbols  $B_{k_A}^1$  and  $B_{-k_A}^1$  express wave function

$$\psi_{B^1}(x) = B^1_{k_B} e^{ik_B x} + B^1_{-k_B} e^{-ik_B x}, \qquad (47)$$

in medium A of second period, the symbols  $A_{k_A}^2$  and  $A_{-k_A}^2$  express wave function

$$\psi_{A^2}(x) = A_{k_A}^2 e^{ik_A x} + A_{-k_A}^2 e^{-ik_A x}, \qquad (48)$$

similarly, in medium *B* of second period, the symbols  $B_{k_A}^2$ and  $B_{-k_A}^2$  express wave function

$$\psi_{B^2}(x) = B_{k_B}^2 e^{ik_B x} + B_{-k_B}^2 e^{-ik_B x}, \qquad (49)$$

$$Fe^{i\mathbf{k}\mathbf{x}} \xrightarrow{f'e^{-i\mathbf{k}\mathbf{x}}} \begin{bmatrix} A_{k_{A}}^{1} & B_{k_{g}}^{1} & A_{k_{A}}^{2} & B_{k_{g}}^{2} \\ A_{-k_{A}}^{1} & B_{-k_{g}}^{1} & A_{-k_{A}}^{2} & B_{-k_{g}}^{2} \end{bmatrix} \cdots \begin{bmatrix} A_{k_{A}}^{N} & B_{k_{g}}^{N} \\ A_{-k_{A}}^{N} & B_{-k_{g}}^{N} \end{bmatrix} \xrightarrow{De^{i\mathbf{k}\mathbf{x}}} \xrightarrow{De^{i\mathbf{k}\mathbf{x}}}$$

Figure 3. The wave method structure  $(AB)^N$  of 1D PCs.

and so on.

In the incident area, the total wave function  $\psi_{tot}(x)$  is the superposition of incident and reflection wave function, it is where K is the wave vector of incident, reflection, and transmission photon. In the following, we should use the condition of wave function and its derivative continuation at interface of two mediums.

(1) At x = 0, by the continuation of wave function and its derivative, we have

$$F + F' = A_{k_A}^1 + A_{-k_A}^1, \tag{50}$$

$$iKF - iKF' = ik_A A^1_{k_A} - ik_A A^1_{-k_A}, \qquad (51)$$

we obtain

$$A_{k_A}^1 = \frac{1}{2} \left[ \left( 1 + \frac{K}{k_A} \right) F + \left( 1 - \frac{K}{k_A} \right) F' \right], \quad (52)$$
$$A_{-k_A}^1 = \frac{1}{2} \left[ \left( 1 - \frac{K}{k_A} \right) F + \left( 1 + \frac{K}{k_A} \right) F' \right], \quad (53)$$

the Equations (53) and (54) can be written as matrix form

$$\begin{pmatrix} A_{k_A}^1\\A_{-k_A}^1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1+K/k_A & 1-K/k_A\\1-K/k_A & 1+K/k_A \end{pmatrix} \begin{pmatrix} F\\F' \end{pmatrix}$$
$$= M_A^1 \begin{pmatrix} F\\F' \end{pmatrix},$$
(54)

where  $M_A^1$  is the wave transfer matrix of the first period medium A, it is

$$M_A^1 = \frac{1}{2} \begin{pmatrix} 1 + K/k_A & 1 - K/k_A \\ 1 - K/k_A & 1 + K/k_A \end{pmatrix},$$
 (55)

(2) At x = a, by the continuation of wave function and its derivative, we have

$$A_{k_{A}}^{1}e^{ik_{A}a} + A_{-k_{A}}^{1}e^{-ik_{A}a} = B_{k_{B}}^{1}e^{ik_{B}a} + B_{-k_{B}}^{1}e^{-ik_{B}a}, \quad (56)$$

$$\frac{k_{A}}{k_{B}}\left(A_{k_{A}}^{1}e^{ik_{A}a} - A_{-k_{A}}^{1}e^{-ik_{A}a}\right) = B_{k_{B}}^{1}e^{ik_{B}a} - B_{-k_{B}}^{1}e^{-ik_{B}a}, \quad (57)$$

we get

$$B_{k_B}^{1} = \frac{1}{2} e^{i(k_A - k_B)a} \left( 1 + \frac{k_A}{k_B} \right) A_{k_A}^{1} + \frac{1}{2} e^{-i(k_A + k_B)a} \left( 1 - \frac{k_A}{k_B} \right) A_{-k_A}^{1}, \quad (58)$$
$$B_{-k_B}^{1} = \frac{1}{2} e^{i(k_A + k_B)a} \left( 1 - \frac{k_A}{k_B} \right) A_{k_A}^{1} + \frac{1}{2} e^{i(k_B - k_A)a} \left( 1 + \frac{k_A}{k_B} \right) A_{-k_A}^{1}, \quad (59)$$

the Equations (59) and (60) can be written as matrix form

$$\begin{pmatrix} B_{k_B}^1 \\ B_{-k_B}^1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} e^{i(k_A - k_B)a}(1 + k_A/k_B) & e^{-i(k_A + k_B)a}(1 - k_A/k_B) \\ e^{i(k_A + k_B)a}(1 - k_A/k_B) & e^{i(k_B - k_A)a}(1 + k_A/k_B) \end{pmatrix} \times \begin{pmatrix} A_{k_A}^1 \\ A_{-kA}^1 \end{pmatrix} = M_B^1 \begin{pmatrix} A_{k_A}^1 \\ A_{-kA}^1 \end{pmatrix},$$
(60)

where  $M_B^1$  is the wave transfer matrix of the first period medium *B*, it is

$$M_B^1 = \frac{1}{2} \begin{pmatrix} e^{i(k_A - k_B)a}(1 + k_A/k_B) & e^{-i(k_A + k_B)a}(1 - k_A/k_B) \\ e^{i(k_A + k_B)a}(1 - k_A/k_B) & e^{i(k_B - k_A)a}(1 + k_A/k_B) \end{pmatrix}$$
(61)  
$$\psi_{tot}(x) = \psi_I(x) + \psi_R(x) = F e^{iKx} + F' e^{-iKx},$$
(62)

(3) At x = a + b, by the continuation of wave function and its derivative, we have

$$B_{k_B}^{1} e^{ik_B(a+b)} + B_{-k_B}^{1} e^{-ik_B(a+b)}$$
  
=  $A_{k_A}^{2} e^{ik_A(a+b)} + A_{-k_A}^{2} e^{-ik_A(a+b)}$ , (63)  
 $k_B \left( p_1 - \frac{ik_B(a+b)}{2} - p_1 - \frac{-ik_B(a+b)}{2} \right)$ 

$$\frac{1}{k_A} \left( B_{k_B} e^{-b(a+b)} - B_{-k_B} e^{-b(a+b)} \right)$$
$$= A_{k_A}^2 e^{ik_A(a+b)} - A_{-k_A}^2 e^{-ik_A(a+b)}, \qquad (64)$$

we get

$$A_{k_{A}}^{2} = \frac{1}{2} e^{i(k_{B}-k_{A})(a+b)} \left(1 + \frac{k_{B}}{k_{A}}\right) B_{k_{B}}^{1} + \frac{1}{2} e^{-i(k_{A}+k_{B})(a+b)} \left(1 - \frac{k_{B}}{k_{A}}\right) B_{-k_{B}}^{1}, \quad (65)$$
$$A_{-k_{A}}^{2} = \frac{1}{2} e^{i(k_{A}+k_{B})(a+b)} \left(1 - \frac{k_{B}}{k_{A}}\right) B_{k_{B}}^{1} + \frac{1}{2} e^{i(k_{A}-k_{B})(a+b)} \left(1 + \frac{k_{B}}{k_{A}}\right) B_{-k_{B}}^{1}, \quad (66)$$

the Equations (65) and (66) can be written as matrix form

$$\begin{pmatrix} A_{k_A}^2 \\ A_{-k_A}^2 \end{pmatrix} = \frac{1}{2} \times \begin{pmatrix} e^{i(k_B - k_A)(a+b)}(1+k_B/k_A) & e^{-i(k_A + k_B)(a+b)}(1-k_B/k_A) \\ e^{i(k_A + k_B)(a+b)}(1-k_B/k_A) & e^{i(k_A - k_B)(a+b)}(1+k_B/k_A) \end{pmatrix} \times \begin{pmatrix} B_{kB}^1 \\ B_{-kB}^1 \end{pmatrix} = M_A^2 \begin{pmatrix} B_{kB}^1 \\ B_{-kB}^1 \end{pmatrix},$$
(67)

where  $M_A^2$  is the wave transfer matrix of the second period medium A, it is

$$\begin{split} M_A^2 &= \frac{1}{2} \\ &\times \begin{pmatrix} e^{i(k_B - k_A)(a+b)}(1 + k_B/k_A) & e^{-i(k_A + k_B)(a+b)}(1 - k_B/k_A) \\ e^{i(k_A + k_B)(a+b)}(1 - k_B/k_A) & e^{i(k_A - k_B)(a+b)}(1 + k_B/k_A) \end{pmatrix}, \end{split}$$
(68)

(4) at x = 2a + b, by the continuation of wave function and its derivative, we get

$$\begin{pmatrix} B_{k_B}^2 \\ B_{-k_B}^2 \end{pmatrix} = \frac{1}{2} \times \begin{pmatrix} e^{i(k_A - k_B)(2a+b)}(1 + k_A/k_B) & e^{-i(k_A + k_B)(2a+b)}(1 - k_A/k_B) \\ e^{i(k_A + k_B)(2a+b)}(1 - k_A/k_B) & e^{i(k_B - k_A)(2a+b)}(1 + k_A/k_B) \end{pmatrix} \times \begin{pmatrix} A_{k_A}^2 \\ A_{-k_A}^2 \end{pmatrix} = M_B^2 \begin{pmatrix} A_{k_A}^2 \\ A_{-k_A}^2 \end{pmatrix},$$
(69)

where  $M_B^2$  is the wave transfer matrix of the second period medium *B*, it is

$$\begin{split} M_B^2 &= \frac{1}{2} \\ &\times \left( \begin{array}{c} e^{i(k_A - k_B)(2a+b)}(1+k_A/k_B) & e^{-i(k_A + k_B)(2a+b)}(1-k_A/k_B) \\ e^{i(k_A + k_B)(2a+b)}(1-k_A/k_B) & e^{i(k_B - k_A)(2a+b)}(1+k_A/k_B) \end{array} \right), \end{split}$$
(70)

(5) at x = 2(a+b), by the continuation of wave function and its derivative, we get

$$\begin{pmatrix} A_{k_A}^3 \\ A_{-k_A}^3 \end{pmatrix} = \frac{1}{2} \times \begin{pmatrix} e^{i(k_B - k_A)2(a+b)}(1 + k_B/k_A) & e^{-i(k_A + k_B)2(a+b)}(1 - k_B/k_A) \\ e^{i(k_A + k_B)2(a+b)}(1 - k_B/k_A) & e^{i(k_A - k_B)2(a+b)}(1 + k_B/k_A) \end{pmatrix} \times \begin{pmatrix} B_{k_B}^2 \\ B_{-k_B}^2 \end{pmatrix} = M_A^3 \begin{pmatrix} B_{k_B}^2 \\ B_{-k_B}^2 \end{pmatrix},$$
(71)

where  $M_A^3$  is the wave transfer matrix of the third period medium A, it is

$$M_A^3 = \frac{1}{2} \times \begin{pmatrix} e^{i(k_B - k_A)2(a+b)}(1+k_B/k_A) & e^{-i(k_A + k_B)2(a+b)}(1-k_B/k_A) \\ e^{i(k_A + k_B)2(a+b)}(1-k_B/k_A) & e^{i(k_A - k_B)2(a+b)}(1+k_B/k_A) \end{pmatrix}$$
(72)

(6) similarly, at x = 3a + 2b, by the continuation of wave function and its derivative, we get

$$\begin{pmatrix} B_{k_B}^3 \\ B_{-k_B}^3 \end{pmatrix} = \frac{1}{2} \times \begin{pmatrix} e^{i(k_A - k_B)(3a + 2b)}(1 + k_A/k_B) & e^{-i(k_A + k_B)(3a + 2b)}(1 - k_A/k_B) \\ e^{i(k_A + k_B)(3a + 2b)}(1 - k_A/k_B) & e^{i(k_B - k_A)(3a + 2b)}(1 + k_A/k_B) \end{pmatrix}$$

$$\times \begin{pmatrix} A_{k_A}^3 \\ A_{k_A}^3 \end{pmatrix} = M^3 \begin{pmatrix} A_{k_A}^3 \\ A_{k_A}^3 \end{pmatrix}$$
(72)

$$\times \begin{pmatrix} \Lambda_{kA} \\ A_{-kA}^3 \end{pmatrix} = M_B^3 \begin{pmatrix} \Lambda_{kA} \\ A_{-kA}^3 \end{pmatrix}, \tag{73}$$

where  $M_B^3$  is the wave transfer matrix of the third period medium *B*, it is

$$\begin{split} M_B^3 &= \frac{1}{2} \\ &\times \begin{pmatrix} e^{i(k_A - k_B)(3a+2b)}(1 + k_A/k_B) & e^{-i(k_A + k_B)(3a+2b)}(1 - k_A/k_B) \\ e^{i(k_A + k_B)(3a+2b)}(1 - k_A/k_B) & e^{i(k_B - k_A)(3a+2b)}(1 + k_A/k_B) \end{pmatrix}. \end{split}$$

$$(74)$$

By the above calculation, we can obtain the results of transfer matrixes:

(1) For the transfer matrix  $M_A^1$  of the first period, medium A is independent form. (2) For the transfer matrixes  $M_A^N$  of



Figure 4. Comparing wave method dispersion relation (*a*) with transfer matrix dispersion relation (*b*).



Figure 5. Comparing wave method transmissivity (a) with transfer matrix transmissivity (b).

the *N*th period  $(N \ge 2)$ , they can be written as:

$$\begin{split} \mathcal{M}_{A}^{N} &= \frac{1}{2} \\ \times \begin{pmatrix} e^{i(k_{B}-k_{A})(N-1)(a+b)}(1+k_{B}/k_{A}) & e^{-i(k_{A}+k_{B})(N-1)(a+b)}(1-k_{B}/k_{A}) \\ e^{i(k_{A}+k_{B})(N-1)(a+b)}(1-k_{B}/k_{A}) & e^{i(k_{A}-k_{B})(N-1)(a+b)}(1+k_{B}/k_{A}) \end{pmatrix}, \end{split}$$

$$(75)$$

(3) For the transfer matrixes  $M_B^N$  of the *N*th period ( $N \ge 1$ ), they can be written as:

$$M_B^N = \frac{1}{2} \times \begin{pmatrix} e^{i(k_A - k_B)(N(a+b)-b)}(1 + k_A/k_B) & e^{-i(k_A + k_B)(N(a+b)-b)}(1 - k_A/k_B) \\ e^{i(k_A + k_B)(N(a+b)-b)}(1 - k_A/k_B) & e^{i(k_B - k_A)(N(a+b)-b)}(1 + k_A/k_B) \end{pmatrix}.$$
(76)



Figure 6. Comparing wave method transmissivity (a) with transfer matrix transmissivity (b).



Figure 7. Comparing wave method transmissivity (a) with transfer matrix transmissivity (b) for the structure  $(AB)^4 D (AB)^4$ .

By the wave transfer matrixes, we can give their relations: (1) The representation of the first period wave transfer matrixes are

$$\begin{pmatrix} A_{k_A}^1 \\ A_{-k_A}^1 \end{pmatrix} = M_A^1 \begin{pmatrix} F \\ F' \end{pmatrix},$$

$$\begin{pmatrix} B_{k_B}^1 \\ B_{-k_B}^1 \end{pmatrix} = M_B^1 \begin{pmatrix} A_{k_A}^1 \\ A_{-k_A}^1 \end{pmatrix} = M_B^1 M_A^1 \begin{pmatrix} F \\ F' \end{pmatrix} = M^1 \begin{pmatrix} F \\ F' \end{pmatrix}.$$

$$(77)$$



Figure 8. Comparing wave method transmissivity (a) with transfer matrix transmissivity (b) for the structure  $(AB)^4 D^2 (AB)^4$ .

(2) The representation of the second period wave transfer matrixes are

$$\begin{pmatrix} A_{k_A}^2 \\ A_{-k_A}^2 \end{pmatrix} = M_A^2 \begin{pmatrix} B_{k_B}^1 \\ B_{-k_B}^1 \end{pmatrix}$$

$$= M_A^2 M_B^1 M_A^1 \begin{pmatrix} F \\ F' \end{pmatrix} = M_A^2 M^1 \begin{pmatrix} F \\ F' \end{pmatrix}, \quad (79)$$

$$\begin{pmatrix} B_{k_B}^2 \\ B_{-k_B}^2 \end{pmatrix} = M_B^2 \begin{pmatrix} A_{k_A}^2 \\ A_{-k_A}^2 \end{pmatrix}$$

$$= M_B^2 M_A^2 M_B^1 M_A^1 \begin{pmatrix} F \\ F' \end{pmatrix} = M^2 M^1 \begin{pmatrix} F \\ F' \end{pmatrix}. \quad (80)$$

(3) Similarly, the representation of the Nth period wave transfer matrixes are

$$\begin{pmatrix} A_{k_A}^N \\ A_{-k_A}^N \end{pmatrix} = M_A^N M_B^{N-1} M_A^{N-1} \cdots M_A^2 M_B^1 M_A^1 \begin{pmatrix} F \\ F' \end{pmatrix}$$
$$= M_A^N M^{N-1} \cdots M^2 M^1 \begin{pmatrix} F \\ F' \end{pmatrix}, \qquad (81)$$
$$\begin{pmatrix} B_{k_B}^N \\ B_{-k_B}^N \end{pmatrix} = M_B^N M_A^N M_B^{N-1} M_A^{N-1} \cdots M_A^2 M_B^1 M_A^1 \begin{pmatrix} F \\ F' \end{pmatrix}$$
$$= M^N M^{N-1} \cdots M^2 M^1 \begin{pmatrix} F \\ F' \end{pmatrix} = M \begin{pmatrix} F \\ F' \end{pmatrix}, \qquad (92)$$

where

(78)

$$M = M^{N} M^{N-1} \cdots M^{2} M^{1} = \begin{pmatrix} m_{1} & m_{2} \\ m_{3} & m_{4} \end{pmatrix}, \quad (83)$$

(82)

is the total wave transfer matrix of N period, and  $M^1 = M_B^1$  $M_A^1$  is the first period wave transfer matrix,  $M^2 = M_B^2 M_A^2$  is



Figure 9. Comparing wave method transmissivity (a) with transfer matrix transmissivity (b) for the structure  $(AB)^4 D_1 D_2 (AB)^4$ .

the second period wave transfer matrix, and  $M^N = M_B^N M_A^N$  is the *N*th period wave transfer matrix.

By Equations (82) and (83), we can give the wave function of Nth period in medium B, it is

$$\psi_B^N(x) = B_{kB}^N e^{ik_B x} + B_{-kB}^N e^{-ik_B x}$$
  
=  $(m_1 F + m_2 F') e^{ik_B x} + (m_3 F + m_4 F') e^{-ik_B x}$   
(84)

In Figure 3, the transmission wave function is

$$\psi_D(x) = De^{iKx}.$$
(85)

At x = N(a+b), by the continuation of wave function and its derivative, we have

$$(m_1F + m_2F') e^{ik_BN(a+b)} + (m_3F + m_4F') e^{-ik_BN(a+b)} = De^{iKN(a+b)},$$
(86)

and

$$\frac{k_B}{K} (m_1 F + m_2 F') e^{ik_B N(a+b)} - \frac{k_B}{K} (m_3 F + m_4 F') e^{-ik_B N(a+b)} = D e^{iKN(a+b)}, \quad (87)$$

we can obtain

$$\frac{F'}{F} = \frac{m_1(K - k_B)e^{ik_BN(a+b)} + m_3(K + k_B)e^{-ik_BN(a+b)}}{m_2(k_B - K)e^{ik_BN(a+b)} - m_4(K + k_B)e^{-ik_BN(a+b)}},$$
(88)

By Equations (86)–(88), we have

$$t = \frac{D}{F} = \left(m_1 + m_2 \frac{F'}{F}\right) e^{i(k_B - K)N(a+b)} + \left(m_3 + m_4 \frac{F'}{F}\right) e^{-i(k_B + K)N(a+b)}, \quad (89)$$

and the wave transmissivity T is

$$T = |t|^2. (90)$$

For the structure  $(AB)^m D(AB)^{N-m}$ , i.e. including the defect layer *D*, its transfer matrix is

$$M_{D} = \frac{1}{2} \times \begin{pmatrix} e^{i(k_{B}-k_{D})m(a+b)}(1+k_{B}/k_{D}) & e^{-i(k_{D}+k_{B})m(a+b)}(1-k_{B}/k_{D}) \\ e^{i(k_{D}+k_{B})m(a+b)}(1-k_{B}/k_{D}) & e^{i(k_{D}-k_{B})m(a+b)}(1+k_{B}/k_{D}) \end{pmatrix}$$
(91)

the total transfer matrix is

$$M = M^{N} M^{N-1} \cdots M_{D} \cdots M^{2} M^{1} = \begin{pmatrix} p_{1} & p_{2} \\ p_{3} & p_{4} \end{pmatrix}, \quad (92)$$

we can obtain the ratio of F'/F including defect layer D, it is

$$\frac{F'}{F} = \frac{p_1(K - k_B)e^{ik_B(N(a+b)+d)} + p_3(K + k_B)e^{-ik_B(N(a+b)+d)}}{p_2(k_B - K)e^{ik_B(N(a+b)+d)} - p_4(K + k_B)e^{-ik_B(N(a+b)+d)}},$$
(93)

where  $k_D = 2\pi n_d / \lambda$ , *d* is the thickness of defect layer *D*, and we have

$$t_D = \frac{D}{F} = \left(p_1 + p_2 \frac{F'}{F}\right) e^{i(k_B - K)(N(a+b)+d)} + \left(p_3 + p_4 \frac{F'}{F}\right) e^{-i(k_B + K)(N(a+b)+d)}, \quad (94)$$

and the wave transmissivity  $T_D$  of including defect layer D, it is

$$T_D = |t|^2. (95)$$

#### 5. Numerical result

In this section, we report our numerical results of the new transmissivity and dispersion relation with and without defect layer. The main parameters are: medium B is  $Na_3AlF_6$ , its refractive indexes is  $n_b = 1.35$ , and its thickness is b = 574 nm. The medium A is GaAs, its refractive indexes is  $n_a = 3.59$ , and its thickness is a = 216 nm. The central frequency is  $\omega_0 = 271 \text{ THz}$ , and the periodicity N = 8. In numerical calculation, we compare the new dispersion relation and transmissivity with the dispersion relation and transmissivity of transfer matrix. With Equation (45), we can calculate the new dispersion relation and compare it with the transfer matrix dispersion relation, which are shown in Figure 4. The Figure 4(a) and (b) are new dispersion relation and transfer matrix dispersion relation, respectively. We can find the two dispersion relation are identical. With Equations (89) and (90), we can calculate the new transmissivity and compare it with transfer matrix transmissivity. In Figure 5(a) and (b) are new transmissivity and transfer matrix transmissivity, respectively. We can find the two transmissivity are identical. In Figure 6, we take the refractive indexes  $n_a = 2.35$ . We can find when the refractive indexes  $n_a$  decrease the band gaps width decrease and the number of band gaps invariant for the two transmissivity, and also find the two kinds of transmissivity 6(a)and 6(b) are identical. With Equations (91) and (95), we can study the structure including defect layer. In Figures 7–9, we consider the effect of defect layer on the transmissivity for the two kinds of calculation results. In Figure 7, the structure is  $(AB)^4 D (AB)^4$ . The defect layer D parameters are: the thickness d = 300 nm, the refractive indexes is  $n_d = 2.58$ . We can find there is a defect mode in the band gap, and the wave method transmissivity 7(a) and the transfer method transmissivity 7(b) are identical. In Figure 8, the structure is  $(AB)^4 D^2 (AB)^4$ , i.e. there are two same defect layers D. We can find there are two defect mode in the band gap, and the wave method transmissivity 8(a) and the transfer method transmissivity 8(b) are identical. In Figure 9, the structure is  $(AB)^4 D_1 D_2 (AB)^4$ , i.e. there are two different defect layers  $D_1$  and  $D_2$ . We can find there are two defect mode in the band gap, and the wave method transmissivity 9(a) and the transfer method transmissivity 9(b) are identical.

#### 6. Conclusion

In the paper, we apply the new wave theory of a photon (from Equation (1) to Equation (10)) in 1D PCs. Since Equation (2) is a partial differential equation, it is difficult to find its solution, so we transfer it into Equations (12) and (13), or Equations (32) and (33) in the alternating media, which are identical with the wave equation of electromagnetic field. With the new wave theory method, we calculate the probability current density of incidence, reflection and transmission. By the continuation of the wave function and its derivative, we provide the new analysis formula of the dispersion relation and transmissivity. In the numerical calculation, we compare the new dispersion relation and transmissivity with those of the TMM. We also find that the dispersion relation and transmissivity with and without the defect layer are identical for the both methods. The new wave method can be also used to study 2D and 3D PCs.

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