Singularity of the Bloch theorem in the fluid/solid phononic crystal

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The physical origin that the plane wave expansion method fails to deal with the fluid/solid phononic crystals is presented. We find that the Bloch theorem is singular in some areas of this kind of system. The unphysical flat bands which appear in the band structure of the fluid/solid systems resulted from the plane wave expansion method can be gotten rid of only when the singularity is removed. As an example, an effective method is presented to calculate the band structure and transmission spectrum of the air/rigid system, in which how to correctly use the Bloch theorem in such kind of systems is shown.

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I. INTRODUCTION

The propagation of elastic or acoustic waves in the so-called phononic crystal (PhC) has received much attention in the last decade.[1–12] In PhCs, the existence of full frequency band gap(s), in which the propagation of elastic waves is forbidden, and some other interesting wave phenomena such as the abnormal refraction[1] should have many potential applications. To understand the elastic or acoustic wave behavior in PhC, several numerical methods such as the plane wave expansion method (PWE),[2] the multiscattering theory (MST),[3] and the finite difference time domain method (FDTD)[4,5] have been developed. Among them, the PWE method, which is based on the Bloch theorem and the Fourier series expansion, is the most popular one in the band structure calculation because of its simplicity and clear physical meaning.

A well-known problem of the PWE method is its numerical convergence. In the practical calculation of the PWE method, a truncating error will be introduced inevitably since only a finite number of the Fourier components can be picked out from the infinite Fourier series. But theoretically, this error can be minimized by using more Fourier components in the expanding expression. Another and more challenging problem for the PWE method, which was encountered in the study of phononic crystal recently, is that it cannot be used in the fluid/solid or inverse structure[5–7] (we denote the system constructed by the separate A phase embedded in the B host as B/A). A lot of unphysical flat bands will appear in the band structure when the PWE method is applied on this kind of systems.[6,7] We know that flat bands in PhCs usually correspond to localized or confined modes, which means the amplitude of these modes is larger in soft material than that in hard material. But for the "unphysical" flat bands, such as the ones appearing in the PWE result of the two-dimensional (2D) Al/Hg lattice,[6] the amplitude of transverse vibrations is finite inside Hg but effectively zero in Al, and this is physically unacceptable. What happens when the PWE method is applied to this kind of system?

From the performance of the PWE method, one would first think that the possible origin of this difficulty is the truncating of the infinite Fourier series, as Garcia-Pablos *et al.* explain that this strange problem is caused by the nonconvergence of the finite Fourier transform of the lame coefficient (μ).[5] But Goffaux and Vigneron[7] show in detail that these flat bands cannot be removed by increasing the plane wave number only. They would appear randomly when the number of plane waves changes. Furthermore, even if one uses the same number of plane waves, the position of the flat bands can vary according to the routines employed in the calculation, so Goffaux and Vigneron conclude that this phenomenon is a "bad numerical problem condition." Moreover, the invalidity of the variational method[8,9] for the fluid/solid system also reveals that this strange problem could not simply contribute to the truncating effect of the Fourier series, because this method is based on the expansion of direct space basis set. Another work that gives this problem an extremely detailed discussion is Ref. 6, where Tanaka *et al.* carefully compare the band structures obtained separately by the FDTD and PWE methods for the Al/Hg lattice. They point out that these flat bands, which are the result of PWE method, are caused by the lack of transverse vibration in fluid, but the physical reason behind it has not been given.

By a detailed investigation we find that this strange problem is caused in fact by the incorrect use of the Bloch theorem. In other words, for the fluid/solid system, some areas are "singular" for the Bloch theorem. We know that the wave solution in a system can take the form of Bloch wave only if two conditions are satisfied. The first one is obviously the periodicity of the considered structure. The second one, which is also apparent but often has been neglected in the application of the PWE method for the PhC calculation, is that in the whole studied system the propagating waves must obey the exact same kind of differential equation. Keeping this in mind, we can find that the Bloch theorem is no longer correct in the fluid/solid or inverse system, because the wave motion in fluid is governed by the *scalar* differential equation, but the wave propagating in solid must satisfy the *full vector* differential equation. We must point out that the wave behaviors governed by these two kind of differential equations are quite different, even though the former equation can be obtained from the latter one by letting the lame coefficient $\mu=0$. In a system consisting of discrete solid material as scatters immersed in fluid host (or inverse), the areas occupied by the scatters are "singular" for the Bloch theorem because the Bloch character of the wave in the host material is broken by them. This singularity must be removed if the Bloch theorem has to be used in this kind of system. For the same reason, we can understand that the Bloch theorem cannot be directly used either in the air/rigid or solid/vaccum (which can be constructed by drilling holes periodically in the solid matrix) system.

A popular numerical method in which the singularity of the Bloch theorem has been removed naturally is MST,[3] where the embedded scatters are considered separately, and a boundary condition is then used to connect the wave solution in the scatters and in the host. The good convergence makes MST one of the best selections in the PhC calculation, but the expansion basic set it used makes this method suitable only for systems with circular or spheroidal shaped scatters.

In Ref. 7, Goffaux and Vigneron suggested but did not prove physically that, in the system with air cavities in solid host, the unphysical flat bands in the PWE result can be got rid of by taking an artificial transverse velocity $c_{t,air}$ in air. From our investigation stated above, we can now understand that the introduction of this artificial transverse velocity makes both conditions required by the Bloch theorem definitely satisfied. In other words, the singularity of the Bloch theorem in the air areas has been removed. But this numerical treatment gives rise to an unreasonable result that the transverse wave can exist in the nonviscous fluid. Moreover, this technique requires the condition $\rho/c_t \rightarrow 0$,[6] where ρ is the mass density, which limits it only applicable to the system with very low-density fluid.

Another structure which has been well studied is the air/solid system.[5,8,10] The solid scatters in this system can be considered as a rigid body because of the huge impedance mismatch between solid and air. To calculate the band structure of this system by the PWE method, the solid scatters have to be looked as fluid materials[5,8,10] to avoid the above-mentioned unphysical modes. This means that the scatters must be absolutely hard to immunize from the excitation of the transverse polarized wave, and at the same time they also should be soft enough to support the longitudinal polarized wave. These two conditions seem very strange, but in fact they suggest again that, to obtain a reasonable result, the singularity of Bloch theorem in scatters must be removed. Although the numerical result under this hypothesis is accurate because the strong wave scattering character of the embedded scatters is kept, the unreasonable hypotheses are physically unacceptable.

In this paper, we take a 2D system as an example to give an alternative method to get rid of the singularity of the Bloch theorem. The chosen system is constructed by the rigid rectangular rods squarely arranged in an air host; the idea can also be used in the solid/vaccum and fluid/solid (or inverse) system. Other systems with circular rods or more complicated shaped scatters can also be dealt with by this method. For the sake of simplicity, only the waves propagating in the xy plane (take $k_z=0$) will be considered. A numerical method, by which the band structure and transmission spectra can be efficiently calculated, is developed accordingly. We can find that in our method the unreasonable conditions needed in the previous works cited above has definitely been abandoned.

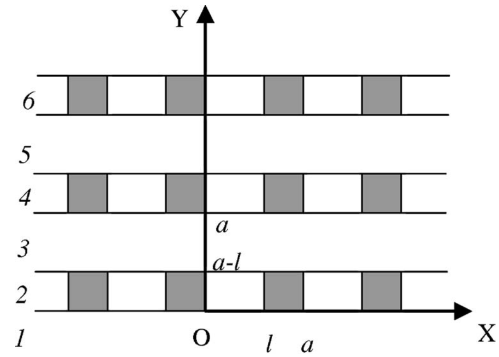

FIG. 1. Birds-eye view of a two-dimensional phononic crystal constructed by rectangular rods (shaded areas) arranged squarely in a uniform host with lattice constant a, l is the distance between two nearest rods. A set of planes parallel to the xoz plane cuts the system into uniform and composite layers along the y direction, which are labeled as $1,3,5,\ldots$ and $2,4,6,\ldots$, respectively.

II. THE CALCULATIONAL METHOD

The considered 2D system shown in Fig. 1 can be cut into two different kinds of layers; one is the uniform layers labeled as 1, 3, 5, etc., and the other one, which is stacked periodically by air and rigid piece, is the composite layers labeled as 2, 4, 6, etc. Following the expression used in Ref. 11, it is easy to write the wave solution in the uniform layers as a superposition of plane wave modes as

$$p(x,y) = \sum_{n=-M}^{+M} e^{i(K_x+G_n)x}[A_n^+ e^{i\beta_n y} + A_n^- e^{-i\beta_n y}] \tag{1}$$

and

$$v_y(x,y) = \sum_{n=-M}^{+M} \frac{\beta_n}{\rho\omega} e^{i(K_x+G_n)x}[A_n^+ e^{i\beta_n y} - A_n^- e^{-i\beta_n y}], \tag{2}$$

where $p(x,y)$ is the pressure field and $v_y(x,y)$ is the velocity field along y direction, ω is the angular frequency of the wave, ρ is the mass density and c is the wave velocity of air, K_x is the Bloch wave vector along the x direction, and A_n^+ and A_n^- are the amplitude of the positive and negative propagating waves along the y direction, respectively. G_n is the reciprocal lattice vector and β_n is the wave number along the y direction, which take the values

$$G_n = 2n\pi/a \ (n = 0, \pm 1, \ldots, \pm M) \tag{3}$$

and

$$\beta_n = \sqrt{(\omega/c)^2 - (K_x + G_n)^2}. \tag{4}$$

In the composite layer, the wave solution can also be written as a superposition of the plane wave modes if it is stacked by two different kinds of fluid or solid materials.[11,12] But in the fluid/solid or solid/vaccum systems, because of the singularity of the Bloch theorem, the expression likes Eqs. (1) and (2) can no longer be used. In the air/rigid system, we note that the wave solution in the composite layers can be expressed as a superposition of the waveguide modes because waves are confined in the air piece. The pressure and velocity field along the y direction can be expressed as

$$p(x,y)=\sum_{n=0}^{N}\cos\frac{n\pi x}{l}[A_n^{+}e^{i\beta_n y}+A_n^{-}e^{-i\beta_n y}] \tag{5}$$

and

$$v_y(x,y)=\sum_{n=0}^{N}\frac{\beta_n}{\rho\omega}\cos\frac{n\pi x}{l}[A_n^{+}e^{i\beta_n y}-A_n^{-}e^{-i\beta_n y}], \tag{6}$$

where

$$\beta_n=\sqrt{\left(\frac{\omega}{c}\right)^2-\left(\frac{n\pi}{l}\right)^2}, \quad (n=0,1,\ldots,N) \tag{7}$$

is the wave vector along the y direction in the air piece.

The wave solutions in the uniform and composite layers can be connected by the boundary condition at the layer interfaces. For the interface between layer k (uniform) and layer $k+1$ (composite), we have

$$p^{(k)}=p^{(k+1)}, \quad 0<x<l, \tag{8}$$

and

$$v_y^{(k)}=\begin{cases} v_y^{(k+1)} & 0<x<l \\ 0 & l<x<a \end{cases}. \tag{9}$$

Substituting Eqs. (1) and (5) into Eq. (8), and using the orthogonality of the waveguide mode, we get

$$\sum_{j=-M}^{+M}M_{mj}^{(k)}(A_j^{(k)+}+A_j^{(k)-})=\sum_{n=0}^{N}M_{mn}^{(k+1)}(A_n^{(k+1)+}+A_n^{(k+1)-}),$$

$$m=0,1,\ldots,N \tag{10}$$

with

$$M_{mj}^{(k)}=\int_0^l\cos\frac{m\pi x}{l}e^{i(K_x+G_j)x}dx, \tag{11}$$

$$M_{mn}^{(k+1)}=\int_0^l\cos\frac{n\pi x}{l}\cos\frac{m\pi x}{l}dx=\begin{cases} 0 & m\neq n \\ l/2 & m=n\neq 0 \\ l & m=n=0 \end{cases}, \tag{12}$$

where the superscripts (k) and $(k+1)$ denote the layer number.

By the same way, we can substitute Eqs. (2) and (6) into Eq. (9), and then get

$$\sum_{j=-M}^{+M}P_{mj}^{(k)}(A_j^{(k)+}-A_j^{(k)-})=\sum_{n=0}^{N}P_{mn}^{(k+1)}(A_n^{(k+1)+}-A_n^{(k+1)-}),$$

$$m=0,\pm 1,\ldots,\pm M \tag{13}$$

with

$$P_{mj}^{(k)}=\begin{cases} a\beta_j^{(k)} & m=j \\ 0 & m\neq j \end{cases}, \tag{14}$$

and

$$P_{mn}^{(k+1)}=\beta_n^{(k+1)}\int_0^l e^{-i(K_x+G_m)x}\cos\frac{n\pi x}{l}dx. \tag{15}$$

Here, the orthogonality of the Fourier components is used.

The matrices $M^{(k)}$, $M^{(k+1)}$, $P^{(k)}$, and $P^{(k+1)}$ should be the square matrices if we set $N+1=2M+1$, and then the linear Eqs. (10) and (13) can be written as

$$\begin{pmatrix} A^{(k+1)+} \\ A^{(k)-} \end{pmatrix}=\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}\begin{pmatrix} A^{(k)+} \\ A^{(k+1)-} \end{pmatrix}, \tag{16}$$

where the matrices

$$S_{22}=2[(M^{(k+1)})^{-1}M^{(k)}+(P^{(k+1)})^{-1}P^{(k)}]^{-1}, \tag{17}$$

$$S_{21}=[(M^{(k+1)})^{-1}M^{(k)}+(P^{(k+1)})^{-1}P^{(k)}]^{-1}[(P^{(k+1)})^{-1}P^{(k)}-(M^{(k+1)})^{-1}M^{(k)}], \tag{18}$$

$$S_{12}=[(M^{(k)})^{-1}M^{(k+1)}+(P^{(k)})^{-1}P^{(k+1)}]^{-1}[(P^{(k)})^{-1}P^{(k+1)}-(M^{(k)})^{-1}M^{(k+1)}], \tag{19}$$

and

$$S_{11}=2[(M^{(k)})^{-1}M^{(k+1)}+(P^{(k)})^{-1}P^{(k+1)}]^{-1} \tag{20}$$

are the so-called scattering matrix.[12,13]

The relationship of the wave amplitudes between the low and upper boundaries of layer k (or $k+1$) can also takes the form of Eq. (16) with

$$S_{12}=S_{21}=0, \tag{21}$$

and

$$S_{11}=S_{22}=\begin{cases} e^{i\beta^k t} & \text{for diagonal terms} \\ 0 & \text{for nondiagonal terms,} \end{cases} \tag{22}$$

where t is the thickness of layer k.

For an infinite system along the y direction, following the idea of the scattering matrix method and using Eqs. (16)–(22), we can get the relationship of the wave amplitudes in the nearest two uniform layers, and then an eigenequation can be obtained if we note that the wave in the uniform layers along the y direction satisfies the Bloch theorem. For a finite system with arbitrary layers, a recursive relation of the wave amplitude in the inputting and outgoing layers can also be obtained by a similar way, by which the transmission and reflection coefficients can be obtained. More details of the scattering matrix method can be found in Refs. 12 and 13.

Before we present our numerical results, it is helpful to briefly discuss other systems. In the 2D solid/vaccum or solid/liquid systems, the elastic wave equation can be divided into two separate equations when only the wave propagating in plane is considered, one of which controls the motion of the xy mode, and the other controls the motion of the z mode. For the z mode, the same formulae presented above can be used if we replace p and v_y by the displacement component u_z and the stress component T_{zy}, respectively. For the xy mode in the solid/vaccum system, the wave modes in the composite layer (it is localized in the solid piece, in fact)

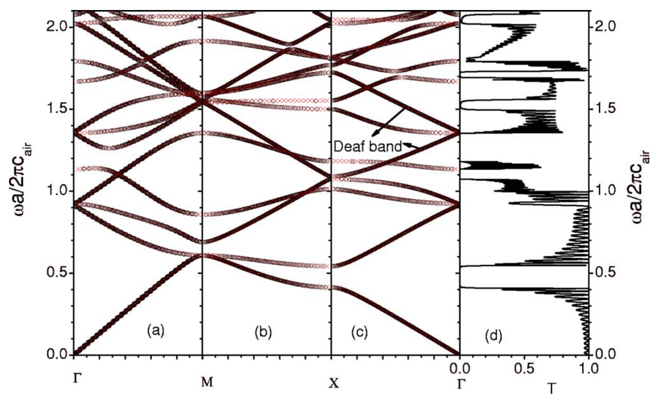

FIG. 2. (Color online) Band structure of the two-dimensional air/rigid system with $f=0.112$ along (a) ΓM, (b) MX, and (c) $X\Gamma$ directions; the circle and cross (red in color) display the results by the our method and by PWE method, respectively. The elastic parameters chosen for the PWE calculations are $\rho_{air}=1\ \text{kgm}^{-3}$, $\rho_{rod}=1500\ \text{kgm}^{-3}$, $c_{air}=340\ \text{ms}^{-1}$, $c_{rod}=2000\ \text{ms}^{-1}$. (d) The transmission coefficient calculated by our method.

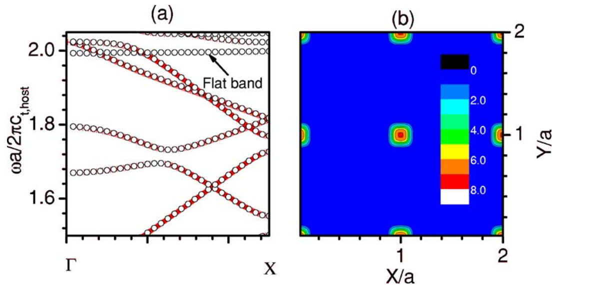

FIG. 3. (Color online) (a) Band structure of z mode of the 2D solid/air system along the ΓX direction with $f=0.112$; results denoted by circle and cross (red in color) are calculated by the PWE and by our method, respectively. A flat band with $\omega a/2\pi c_{t,host}\approx 2$ occurs only in the result of PWE method. Except an artificial $c_{t,air}=1500\ \text{ms}^{-1}$ is used in air, the elastic parameters chosen for PWE calculation are the same as the air/rigid system. (b) Wave amplitude distribution of the flat band at the Γ point, amplitude in two unit cells along the x and y directions is shown.

are the well-known Lamb wave modes, by which the displacement and stress component wave can also be expressed as a superposition in principle, but the normalization condition of the Lamb modes is much more complicated.[14] So, to use our method in this system practically, other basic function sets should be found. As for the solid/liquid system, the circumstance is more complicated because the longitudinal and transverse wave modes in the solid and liquid pieces of the composite layer can be interexcited by each other, and the wave modes in it will have the form of general Lamb modes.[15]

III. RESULT AND DISCUSSION

For the air/rigid system, a typical band structure with volume filling fraction $f=0.112$ obtained by our method is shown by circular dots in Figs. 2(a)–2(c). The results by the traditional PWE method under the hypothesis used in Ref. 8 are also presented by cross symbols. From the pictures we can see that the results from these two methods are overlapped very well. We have used 529 plane wave in the traditional PWE method calculation, but in our present method only nine plane waves (waveguide modes) are needed, which shows the good convergence of our method. The corresponding transmission spectrum (energy flow) for a plane wave incident along ΓX direction of a slab with 16 unit cells is presented in Fig. 2(d). The correspondence [except the deaf bands[8] marked in Fig. 2(c)] between the band in ΓX direction and the transmission spectrum verifies the correctness of our method from another aspect. Note that for this system, no other existing numerical method can be used to calculate the transmission spectrum except the FDTD method.

In the calculation of the z mode band for the solid/vaccum or solid/liquid systems, it is necessary to discuss briefly the approach presented in Ref. 7, in which a sufficient large transverse velocity in air (denoted as $c_{t,air}$ in the following) is introduced to avoid the un-physical flat bands in the PWE method result. In our practical calculation we find that their approach cannot remove the flat bands completely when a high frequency mode is considered. In other words, another kind of flat band would appear in a higher frequency region. A numerical example is presented in Fig. 3(a) when the transverse velocity $c_{t,air}=1500\ \text{ms}^{-1}$ (as chosen in Ref. 7) in air is chosen, where a flat band around $\omega a/2\pi c_{t,host}=2$ appears in the result of PWE method. This flat band should not be caused by the singularity of the Bloch theorem because it has already been removed by introducing a nonzero $c_{t,air}$. To discover what it is, the wave amplitude distribution of this mode at Γ point is presented in Fig. 3(b), where we can see that the vibration is mainly localized in the air holes. It shows that this is a confined mode caused by the imaginary introduced $c_{t,air}$ in air. Obviously, it is another kind of unreasonable mode, and cannot be removed by numerical technique.

Finally, we would like to point out that from the mathematical point of view, the solutions of the elastic equation in the PhC can be determined completely by the Bloch theorem, but it would be overdetermination if an additional boundary condition were to be added. In the fluid/solid or inverse system, the lack of transverse wave in fluid (with the lame coefficient $\mu=0$) implies a boundary condition with zero transverse stress components at the interface of the solid and fluid, so the Bloch theorem can be used only if this boundary condition is revised. In this case we can understand consequently the origin of the "bad numerical problem condition" mentioned in Ref. 7. In this paper, we present an alternative method to remove the singulary of the Bloch theorem. Evidently, our method is much more natural and reasonable.

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