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Band inversion and singularities in one-dimensional phononic crystals

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1. Introduction

Over the past three decades, extensive studies have focused on acoustic waves and phonons in phononic crystals [1]. The distinctive characteristics of phonons in these structures are intrinsically tied to the presence of phononic bandgaps, which arise from Bragg reflections of phonons by the artificially designed periodic structures. In many studies, the band structure was derived by calculating the frequencies of several allowed waves as eigenvalues for a given wave number. In contrast to eigenfrequencies, the detailed characteristics of eigenvectors have only recently begun to receive significant attention.

Meanwhile, topological insulators have gained significant interest in recent years. The concepts utilized in topological insulators have been applied to photonic and phononic crystals [2] after being discovered in electronic systems. In particular, phenomena such as band inversion are discussed based on the eigenvectors of the bands. It is valuable to examine the eigenvectors of phonons in phononic crystals from a fresh perspective. In the present paper, we focus on the band-edge states in one-dimensional phononic crystals and examine the relationship between their symmetry and singularities.

2. Theoretical method

The calculation method we used is based on the transfer matrix method [3]. The displacement and velocity fields are obtained by solving the elastic equation for each layer of the one-dimensional phononic crystal. By applying Bloch's theorem along with boundary conditions that ensure continuity of displacement and stress at the interface, the eigenfrequencies and eigenvectors can be determined.

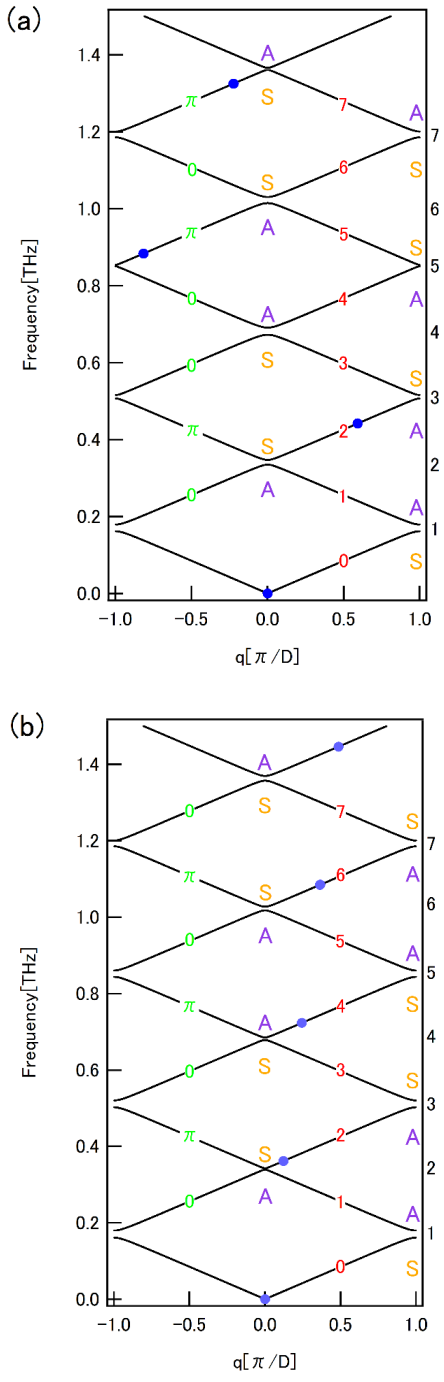

Fig. 1 Phonon dispersion relations for (a) PC1 and (b) PC2. The band indexes are indicated by red numbers, and the gaps are numbered as black numbers. The symmetry at the band edges is marked with S or A, and the blue dots indicate singularities.

3. Numerical results and discussions

Figure 1 shows the phononic band structures calculated for two one-dimensional phononic crystals PC1 and PC2, which are composed of GaAs and AlAs. In PC1 (PC2), the thicknesses of the GaAs and AlAs are assumed to be 8.48 (7.31) nm and 6.39 (7.82) nm, respectively. In PC1 and PC2, the layer thickness is selected to ensure that the center frequency of the gap remains unchanged.

From the components of the calculated eigenvectors, we can examine the symmetry at each band edge of PC1 and PC2, which are marked as S and A in Fig. 1, respectively, depending on whether they are symmetric or antisymmetric. The symmetry of the upper and lower band edges on either side of the band gap is different. This can be explained based on analytical calculations.

On the other hand, there exist bands whose upper and lower edges have the same symmetry and bands whose upper and lower edges have different symmetries. This can be explained topologically using the Zak phase. For the *m*th band, the Zak phase can be defined as

$$\theta_m = \int_{-\pi/D}^{\pi/D} \left[i \int_{\text{unit cell}} u_{m,q}^{*}(x) \frac{\partial}{\partial q} u_{m,q}(x) dx \right] dq \cdot \quad (1)$$

Here, the part in brackets is the Berry connection and $u_{m,q}(x)$ is the periodic part of the Bloch function that represents the displacement field, i.e.,

$$U_{m,q}(x) = e^{iqx} u_{m,q}(x), \quad (2)$$

where q is the Bloch wave number. The Zak phases calculated using Eq.(1) for each band are shown in green in Fig. 1.

The Zak phase defined by Eq. (1) is zero if $u_{m,q}(x)$ is a continuous function of q. On the other hand, it can be shown that it is π if $u_{m,q}(x)$ has a singularity, which are indicated by blue dots in Fig. 1. When the Zak phase of a band is 0, the symmetry is the same at both ends of the band, but it is different for a band with a Zak phase of π.

In PC1, singularities occur in the 2nd, 5th, and 7th bands, while in PC2, they occur in the 2nd, 4th, and 6th bands. The symmetry undergoes changes as one passes through these bands.

Next, in order to investigate the localized modes occurring at the interface of the system in which PC1 and PC2 are connected, the calculated transmittance is shown in Fig. 2. Resonant peaks due to localized modes are observed in the fifth and seventh gaps, which can be understood based on the bulk-edge correspondence.

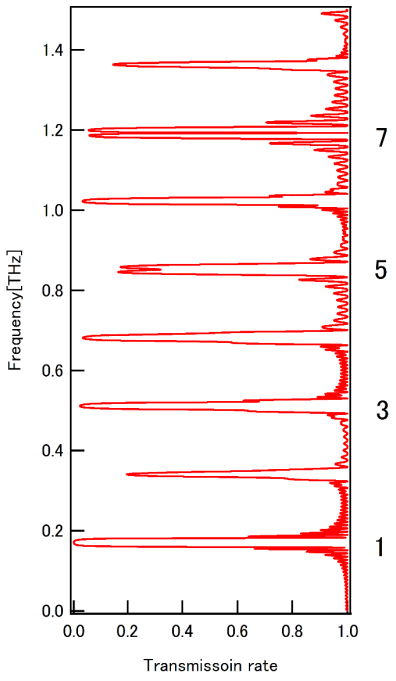

Fig. 2 Transmission spectrum of phonons propagating through a PC1-PC2 junction system. The number of periods in both PC1 and PC2 is chosen to be 10.

Acknowledgment

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References

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