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Band structure of PT-symmetric phononic crystals

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Abstract. In the present paper, the theory of phononic crystals is generalized to the case of periodic media with anisotropic elastic properties, as well as to the PT-symmetric structures with gain and loss. An operator form of the equation for a stationary elastic wave in a crystal is proposed. A generalized condition of PT symmetry for systems with anisotropic elastic properties is obtained.

Keywords: phononic crystal, PT symmetry, exceptional points

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Зонная структура PT-симметричных фононных кристаллов

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Аннотация. В настоящей работе теория фононных кристаллов обобщается на случай периодических сред с анизотропией упругих свойств, а также PT-симметричных структур с усилением и потерями. Предлагается операторная форма записи уравнения стационарной упругой волны в кристалле. Получено обобщенное условие PT-симметрии для систем с анизотропными упругими свойствами.

Ключевые слова: фононный кристалл, PT-симметрия, особые точки

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Introduction

Over the past decade, the properties of parity-time-symmetric (PT-symmetric) systems have been actively studied. Such systems are invariant under the parity (P) and time (T) reversal. The concept of PT symmetry is considered not only in quantum mechanics but also in continuum media theory. In particular, PT symmetry in the theory of elastic waves enables the study of various fundamental phenomena, such as one-way propagation [1], unidirectional sound focusing [2], and invisible sensing [3].

In this context, phononic crystals (PC) are crucial components of the implementation of these effects into the development of novel electronic devices. Most works in the field of PT-symmetric phononic crystals focus on the structures based on isotropic media [1, 4]. However, there is a lack of theoretical investigations of PT-symmetric systems based on semiconductor heterostructures, which often exhibit anisotropic elastic properties.

In the present paper, a general operator formalism for the analysis of elastic waves in a PC is proposed, which allows studying media with arbitrary anisotropy of elastic and mechanical properties. The developed theoretical approach is used to study the band structure of PT-symmetric phononic crystals, taking into account special cases of PT symmetry breaking.

Theory

In the framework of continuum mechanics, stationary elastic waves in crystals are described by the following equation:

$$\sum_{k,l,m} c_{iklm}(\mathbf{x})\frac{\partial^2 u_m(\mathbf{x})}{\partial x_k \partial x_l} = -\omega^2 \mu(\mathbf{x}) u_i(\mathbf{x}), \quad (1)$$

where $c_{iklm}(\mathbf{x})$ is the component of the elasticity tensor, $u_i(\mathbf{x})$ is the complex amplitude of the displacement vector, $\mu(\mathbf{x})$ is the coordinate-dependent crystal density, ω is frequency of elastic waves. Note that considering the displacement field reality, the displacement vector components $\mathbf{u}(\mathbf{x}, t)$ can be expressed through the real part of the corresponding complex phasor $\mathbf{u}(\mathbf{x})e^{-i\omega t}$.

In the general case, a structure under study can be characterized by losses or gain. From a mathematical point of view, such properties of elastic media are described by the imaginary part of the elastic tensor $\tilde{\mathbf{C}}(\mathbf{x})$, which can be represented as:

$$\tilde{\mathbf{C}}(\mathbf{x}) = \tilde{\mathbf{C}}'(\mathbf{x}) + i\tilde{\mathbf{C}}''(\mathbf{x}),$$

where $\tilde{\mathbf{C}}'(\mathbf{x})$ and $\tilde{\mathbf{C}}''(\mathbf{x})$ are its real and imaginary parts, respectively. Note that the complex parameters of the analyzed systems naturally arise when considering time (or spatial) dispersion effects. However, when the components of the elastic tensor change slightly over a given frequency range, it is sufficient to use their constant values. Such a way of description of elastic properties is widely used in the theory of PT-symmetric phononic crystals, where gain and loss are engineered artificially and maintained under certain experimental conditions [1, 2, 4].

Taking into account space inversion and time reversal, we can write a generalized PT symmetry condition for crystal density and elasticity tensor coordinate dependencies:

$$\mu(\mathbf{x}) = \mu(-\mathbf{x}),\ \tilde{\mathbf{C}}(\mathbf{x}) = \tilde{\mathbf{C}}^*(-\mathbf{x}).$$

Note that time reversal reduces to complex conjugation [1].

It can be shown that conventional Eq. (1) is a special case of the following operator equation, written in the coordinate representation:

$$(\hat{\mathbf{s}} \cdot \hat{\mathbf{k}})^+ \hat{c} (\hat{\mathbf{s}} \cdot \hat{\mathbf{k}}) |u\rangle = \omega^2 \hat{\mu} |u\rangle. \quad (2)$$

Here $\hat{\mathbf{s}}$ is the polarization operator, $\hat{\mathbf{k}}$ is the wave vector operator, $\hat{c}$ and $\hat{\mu}$ are the operators of the elasticity and density of the crystal, respectively, $|u\rangle$ is a vector in a complex Hilbert space that describes a displacement field. A similar approach was successfully developed in the theory of photonic crystals [5].

To prove the equivalence of Eqs. (1) and (2), it is necessary to write the operator equation in a certain basis. Consider a set of states "of phonon" $|i, \mathbf{x}\rangle$ with a certain coordinate $\mathbf{x}$ and elastic wave polarization i ($i = x, y, z$). These states form a basis that satisfies the conditions of orthonormality and completeness:

$$\langle i,\mathbf{x}|k,\mathbf{x}'\rangle = \delta(\mathbf{x}-\mathbf{x}')\delta_{ik},\ \langle i,l;\mathbf{x}|k,m;\mathbf{x}'\rangle = \delta(\mathbf{x}-\mathbf{x}')\delta_{ik}\delta_{lm},$$
$$\sum_i \int_V d\mathbf{x}|i,\mathbf{x}\rangle\langle i,\mathbf{x}| = 1,\ \sum_{i,l}\int_V d\mathbf{x}|i,l;\mathbf{x}\rangle\langle i,l;\mathbf{x}| = 1, \tag{3}$$

where V is the volume.

Using this basis set, we can define the vector $|u\rangle$ in coordinate representation:

$$|u\rangle = \sum_i \int_V d\mathbf{x}|i,\mathbf{x}\rangle\langle i,\mathbf{x}|u\rangle = \sum_i \int_V d\mathbf{x}|i,\mathbf{x}\rangle u_i(\mathbf{x}).$$

The matrix elements of the operators in Eq. (2) are determined as follows:

$$\langle i,k;\mathbf{x}|\hat{c}|l,m;\mathbf{x}'\rangle = c_{iklm}(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}'),\ \langle i,\mathbf{x}|\hat{\mu}|k,\mathbf{x}'\rangle = \mu(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}')\delta_{ik},$$
$$\langle i,\mathbf{x}|\hat{\mathbf{k}}|k,\mathbf{x}'\rangle = -i[\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{x}')]\delta_{ik},\ \langle i,l;\mathbf{x}|\hat{\mathbf{s}}|k,\mathbf{x}'\rangle = \mathbf{s}_{il,k}\delta(\mathbf{x}-\mathbf{x}'),$$

where $\mathbf{s}_{il,k}$ are the matrix elements written through the Clebsch–Gordan coefficients [6].

Using expressions (2), (3), it can be shown that:

$$\langle i,k;\mathbf{x}|\hat{c}\left(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}}\right)|u\rangle = \sum_l \int_V d\mathbf{x}'\langle i,k;\mathbf{x}|\hat{c}\left(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}}\right)|l,\mathbf{x}'\rangle\langle l,\mathbf{x}'|u\rangle = \sigma_{ik},$$
$$\langle i;\mathbf{x}|\left(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}}\right)^+|\sigma\rangle = \sum_{l,m}\int_V d\mathbf{x}'\langle i;\mathbf{x}|\left(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}}\right)^+|l,m;\mathbf{x}'\rangle\langle l,m;\mathbf{x}'|\sigma\rangle = \sum_l \frac{\partial\sigma_{il}}{\partial x_l},$$

where σ_{ik} is the component of the mechanical stress tensor and $|\sigma\rangle$ is the corresponding state vector in the complex Hilbert space, describing a mechanical stress field.

Using the relation between the mechanical stress tensor and the strain tensor [6], Eq. (1) can be written in the following form:

$$\sum_k \frac{\partial\sigma_{ik}}{\partial x_k} = -\mu\omega^2 u_i.$$

Thus, Eq. (2) in the coordinate representation reduces to Eq. (1).

By introducing auxiliary vectors $|\tilde{u}\rangle = \hat{\mu}^{1/2}|u\rangle$, we can reduce Eq. (2) to the eigenvalue problem for a non-Hermitian operator:

$$\hat{D}|\tilde{u}\rangle = \omega^2|\tilde{u}\rangle.$$

Here, we introduced a "dynamical" operator $\hat{D} = \hat{\mu}^{-1/2}(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}})^+\hat{c}(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}})\hat{\mu}^{-1/2}$, whose eigenvalues are squared eigenfrequencies.

A phononic crystal is a translationally invariant system with periodically changing elastic properties. In this case, it is convenient to use states with a certain wave vector and polarization as a basis $|i, \mathbf{b} + \mathbf{k}\rangle$ ($\mathbf{b}$ is the reciprocal lattice vector of the PC, $\mathbf{k}$ – the wave vector, taking values in the corresponding superlattice Brillouin zone). Set of states $|i, \mathbf{b} + \mathbf{k}\rangle$ is also considered orthonormal and complete.

The corresponding matrix elements of the operators in Eq. (2) are defined as:

$$\langle i,l;\mathbf{b}+\mathbf{k}|\hat{c}|k,m;\mathbf{b}'+\mathbf{k}'\rangle = c_{iklm}(\mathbf{b}-\mathbf{b}')\delta_{\mathbf{kk}'},\ \langle i,\mathbf{b}+\mathbf{k}|\hat{\mu}|l,\mathbf{b}'+\mathbf{k}'\rangle = \mu(\mathbf{b}-\mathbf{b}')\delta_{il}\delta_{\mathbf{kk}'},$$
$$\langle i,\mathbf{b}+\mathbf{k}|\hat{\mathbf{k}}|l,\mathbf{b}'+\mathbf{k}'\rangle = (\mathbf{b}+\mathbf{k})\delta_{\mathbf{bb}'}\delta_{\mathbf{kk}'}\delta_{il},\ \langle i,l;\mathbf{b}+\mathbf{k}|\hat{\mathbf{s}}|m,\mathbf{b}'+\mathbf{k}'\rangle = \mathbf{s}_{il,m}\delta_{\mathbf{bb}'}\delta_{\mathbf{kk}'}, \tag{4}$$

where $c_{iklm}(\mathbf{b} - \mathbf{b}')$ and $\mu(\mathbf{b} - \mathbf{b}')$ are the Fourier transforms of the components of the elastic tensor and the crystal density, respectively.

Expressions (4) allow determining the matrix of the operator $\hat{D}$, which is diagonal in indices **k** and **k'** and has a block-diagonal structure, where each block is a matrix of smaller dimension, corresponding to a certain value of the vector **k**. As a consequence, the operator Eq. (2) can be represented as the following matrix equation:

$$D(\mathbf{k})\tilde{\mathbf{u}}_j(\mathbf{k}) = \omega_j^{\,2}(\mathbf{k})\tilde{\mathbf{u}}_j(\mathbf{k}).$$

Herein $D(\mathbf{k})$ is the matrix of the operator $\hat{D}$, and $\tilde{\mathbf{u}}_j(\mathbf{k})$ are the corresponding eigenvectors.

Thus, the problem of determining the band structure of a phononic crystal is reduced to the problem of determining the eigenvalues $\omega_j^2(\mathbf{k})$ and eigenvectors $\tilde{\mathbf{u}}_j(\mathbf{k})$ of a non-Hermitian matrix. It should be noted that in a non-Hermitian problem, the eigenvectors are not orthogonal, but are related by the conditions of biorthonormality and completeness to the solution of the adjoint problem for eigenvalues and eigenvectors [7].

To determine the spatial distribution of the displacement field, it is necessary to consider $\tilde{\mathbf{u}}_j(\mathbf{k})$ in the basis $|i, \mathbf{x}\rangle$, which is related to the basis $|i, \mathbf{b} + \mathbf{k}\rangle$ by the inverse Fourier transform:

$$u_{i,j}(\mathbf{x};\mathbf{k}) = \frac{1}{\sqrt{\Omega}}\sum_{\mathbf{b}} e^{i\mathbf{bx}} u_{\mathbf{b}i,j}(\mathbf{k}).$$

Here Ω is the volume of a unit cell. Components $u_{\mathbf{b}i,j}(\mathbf{k})$ form respective vectors $\mathbf{u}_j(\mathbf{k})$, which are related to the eigenvectors $\tilde{\mathbf{u}}_j(\mathbf{k})$ of the matrix $D(\mathbf{k})$ by the following formula:

$$\mathbf{u}_j(\mathbf{k}) = \mu^{-1/2}\tilde{\mathbf{u}}_j(\mathbf{k}),$$

where the matrix μ is defined through the matrix elements (4).

Results and Discussion

The theory developed was used to analyze the band structure and the displacement fields of a one-dimensional PT-symmetric anisotropic PC. The studied structure is schematically shown in Fig. 1. The values of the elasticity tensor components were taken from [8, 9].

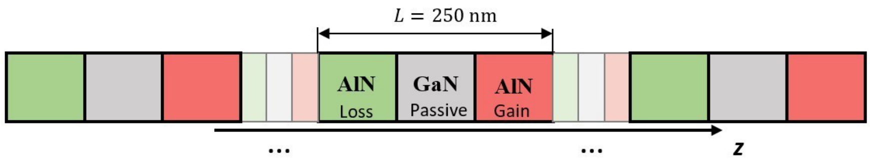

Fig. 1. One-dimensional PC consisting of AlN/GaN layers. The PC period is L = 250 nm. Passive regions are marked in gray, regions characterizing wave amplification are marked in red, and attenuation is marked in green

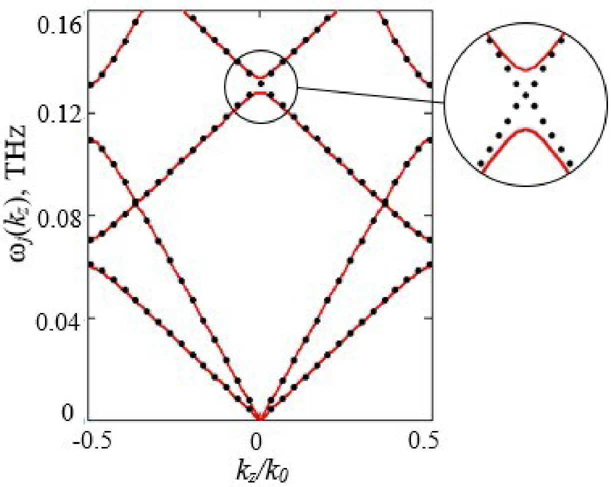

Fig. 2. Band structure of passive PC (red line) and PT-symmetric PC (black dotted line ($\gamma = 2$))

The energy loss and gain in AlN cells are characterized by the following imaginary components of the elasticity tensor: $c''_{11} = c''_{44} = \pm\gamma \cdot 10^{10}$ Pa (where "+" denotes a cell with loss, "–" denotes a cell with gain). Fig. 2 shows the calculated band structure of the fully passive 1D AlN/GaN PC (without gain and loss), as well as a PT-symmetric 1D PC with active elementary cells.

As can be seen from Fig. 2, the band structures for the passive PC and the PT-symmetric PC slightly differ quantitatively. However, a coalescence of the dispersion branches can be observed for the latter case. Fig. 3, *a* shows the spatial distribution of the displacement fields for a PC with PT symmetry and its violation (Fig. 3, *b*).

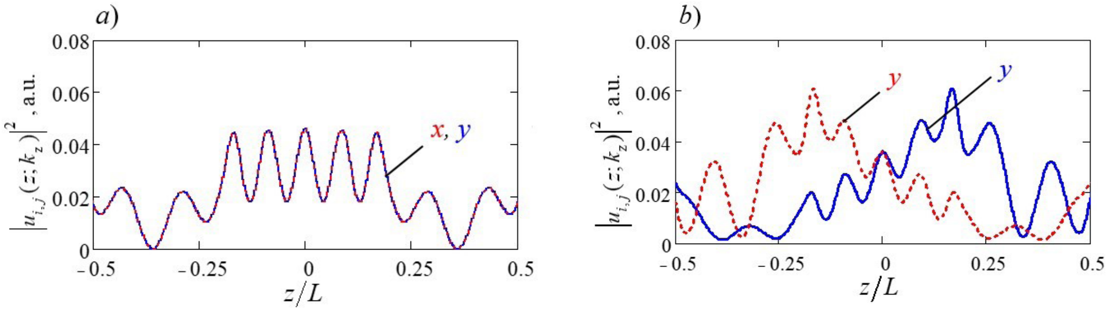

Fig. 3. Squared modulus of displacement fields at $k_z = 0.25k_0$, $j = 21$, $i = x$ (red dotted line), and at $j = 22$, $i = y$ (blue line), PT-symmetric case ($\gamma = 6$) (*a*); squared modulus of the displacement fields at $k_z = 0.25k_0$, $j = 21$, $i = y$ (red dotted line), and at $j = 22$, $i = y$ (blue line), case of PT symmetry breaking ($\gamma = 7$) (*b*). $k_0 = 2\pi/L$.

One of the characteristic features of PT-symmetric systems is the presence of exceptional points, corresponding to singularities in the dependence of frequency on the system parameters. Fig. 4 shows the dependencies of the imaginary frequency component for two modes $j = 21$, 22 on the parameter γ.

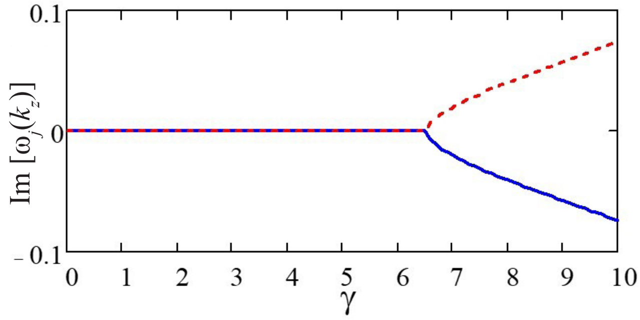

Fig. 4. Dependences of imaginary frequency component for two modes $j = 21$ (red dotted line) and $j = 22$ (blue line) on the parameter γ, for $k_z = 0.25k_0$

Fig. 4 shows an exceptional point for $\gamma \approx 6.5$, corresponding to the broken PT symmetry. This explains that when $\gamma = 6$ (Fig. 3, *a*) the amplitudes of the waves in the regions with gain and loss are equal, while for the case $\gamma = 7$ (Fig. 3, *b*) such symmetry of the eigenstates cannot be observed.

Conclusion

The paper develops a new theoretical approach for the analysis of the band structure of the phononic crystal. A generalized operator form of the equation of a stationary elastic wave in a crystal is proposed. It is shown that the problem of determining the band structure and eigenmodes of a PC is reduced to a matrix problem of finding eigenvalues and eigenvectors. This approach allows analyzing the PCs with arbitrary anisotropy of elastic properties. A generalized condition for PT-symmetric systems with anisotropic elastic properties was obtained. The proposed method was used to calculate the band structure and the spatial distribution of the displacement field of the one-dimensional PT-symmetric PC and to analyze the system's behavior near the exceptional points. This theory can be further developed to study systems with temporal and spatial dispersion of elastic properties, analogous to the operator formalism of macroscopic electrodynamics [7].

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