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Band-Gap Structure of the Spectrum of Periodic Maxwell Operators

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We investigate the band-gap structure of some second-order differential operators associated with the propagation of waves in periodic two-component media. Particularly, the operator associated with the Maxwell equations with position-dependent dielectric constant $\varepsilon(x)$, $x \in \mathbf{R}^3$, is considered. The medium is assumed to consist of two components: the background, where $\varepsilon(x) = \varepsilon_b$, and the embedded component composed of periodically positioned disjoint cubes, where $\varepsilon(x) = \varepsilon_a$. We show that the spectrum of the relevant operator has gaps provided some reasonable conditions are imposed on the parameters of the medium. Particularly, we show that one can open up at least one gap in the spectrum at any preassigned point λ provided that the size of cubes L, the distance $l = \delta L$ between them, and the contrast $\varepsilon = \varepsilon_b/\varepsilon_a$ are chosen in such a way that $L^{-2} \sim \lambda$, and quantities $\varepsilon^{-1}\delta^{-3/2}$ and $\varepsilon\delta^2$ are small enough. If these conditions are satisfied, the spectrum is located in a vicinity of width $w \sim (\varepsilon\delta^{3/2})^{-1}$ of the set $\{\pi^2 L^{-2} k^2 : k \in \mathbf{Z}^3\}$. This means, in particular, that any finite number of gaps between the elements of this discrete set can be opened simultaneously, and the corresponding bands of the spectrum can be made arbitrarily narrow. The method developed shows that if the embedded component consists of periodically positioned balls or other domains which cannot pack the space without overlapping, one should expect pseudogaps rather than real gaps in the spectrum.

KEY WORDS: Waves; periodic dielectrics; periodic acoustic media; gaps in the spectrum.

1. INTRODUCTION

The idea of finding and designing periodic dielectric materials which exhibit gaps in the spectrum was introduced quite recently.[1,2] The general reason

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for the rise of gaps lies in the coherent multiple scattering and interference of waves (see, for instance, John[3] and references therein). The experimental results[4-6] for periodic and disordered dielectrics indicate that the photonic gap regime can be achieved for some nonhomogeneous materials. The analysis of some approximate models and the numerical computations[7-11] have shown the possibility of a gap (or pseudogap) regime for some two-component periodic dielectrics. The most recent theoretical and experimental achievements in the investigation of the photonic band-gap structures are published in the series of papers in ref. 12.

To study the properties of wave propagation in a nonhomogeneous medium one has to investigate the spectral properties of the relevant self-adjoint differential operators with coefficients varying in space. Such an operator for electromagnetic waves has the form

$$\Lambda\Psi = \nabla \times (\gamma(x)\nabla \times \Psi), \qquad \nabla \cdot \Psi = 0, \qquad \gamma(x) = \varepsilon^{-1}(x), \qquad x \in \mathbf{R}^3 \quad (1)$$

where $\Psi(x)$ is a complex vector function on $\mathbf{R}^3$. The important analog of this operator is the following operator of second order acting on the space of complex scalar-valued functions $\psi(x)$ on $\mathbf{R}^3$:

$$\Gamma\psi = -\sum_{j=1}^{3} \frac{\partial}{\partial x_j}\gamma(x)\frac{\partial}{\partial x_j}\psi, \qquad x \in \mathbf{R}^3 \quad (2)$$

It can be associated with the propagation of acoustic waves. In the first formula $\varepsilon(x)$ stands for the electric permittivity for electromagnetic waves, whereas for acoustic waves it stands for the mass density of the medium. The coefficient $\varepsilon(x)$, $x \in \mathbf{R}^3$, that we consider here is a periodic function bounded from above and below by positive constants. The important parameters of such a two-component periodic medium that can shape the spectrum[6] are the volume-filling fraction, the dielectric constant contrast $\varepsilon_b/\varepsilon_a$ (where ε_b and ε_a are, respectively, the dielectric constants of the host material and the embedded components), and the shape of atoms of the embedded material as well as their arrangement. In particular, the high dielectric constant contrast favors the rise of gaps in the spectrum (some living tissues possess very high contrast[13]).

We show here the existence of gaps under certain conditions for two-component dielectrics, which can be thought of as bubbles of air embedded in an optically dense background. The existence of gaps for the lattice (finite-difference) version of the relevant operators and the existence of pseudogaps for operators Λ and Γ have been already established[14,15] (in particular, the limit location of the bands of the spectrum was found[15] under the assumption that the contrast in dielectric constants between the background and the embedded component approaches infinity). Our analysis shows that to open up a gap in a preassigned point of the spectrum one has to provide certain quite simple relationships between the geometric parameters of the periodic arrangement of bubbles (which are assumed to be just cubes) and the contrast in the dielectric constant.

2. STATEMENT OF RESULTS AND SKETCH OF THE PROOF

The operators of interest are the operators Λ and Γ defined above. We begin with a construction of such a dielectric medium in the space $\mathbf{R}^3$ for which the dielectric permittivity $\varepsilon(x)$, $x \in \mathbf{R}^3$, equals 1 on a set of disjoint bounded finite domains (a sort of air bubbles) spread in the space, and it takes on a constant value grater than 1 in the rest of the space, which we call the background, so $\varepsilon(x) > 1$ there. We will be interested in the case when ε tends to infinity on the background, that is, in the medium with a high contrast between the background and the bubbles.

We suppose that the space $\mathbf{R}^3$ is packed periodically without overlapping by the cubes O_α:

$$O_\alpha = O + L\alpha, \qquad \alpha \in \mathbf{Z}^3$$

$$O = \{x = (x_1, x_2, x_3) \in \mathbf{R}^3 \colon \delta L \leqslant x_j \leqslant (1-\delta)\, L,\ 1 \leqslant j \leqslant 3\}$$

$$0 < 2\delta < 1$$

where $2\delta L$ is the distance between adjacent cubes O_α. The union of O_α is denoted by $\mathscr{A}$, and its complimentary set, which forms the background, is denoted by $\mathscr{B}$:

$$\bigcup_{\alpha \in \mathbf{Z}^d} O_\alpha = \mathscr{A}, \qquad O_\alpha \cap O_\beta = \varnothing \quad \text{for} \quad \alpha \neq \beta, \qquad \mathscr{B} = \mathbf{R}^d - \mathscr{A}$$

The boundary ∂O_α of the cube O_α is oriented in standard fashion: the normal vector ν points toward the exterior of O_α. We introduce ε which depends on a parameter $\gamma < 1$ in the following way:

$$\varepsilon = \varepsilon(\gamma, x) = \begin{cases} 1 & \text{if} \quad x \in \mathscr{A} \\ \gamma^{-1} & \text{if} \quad x \in \mathscr{B} \end{cases} \tag{3}$$

Let us denote by σ_L the spectrum of the Laplace operator with zero Neumann boundary conditions on the cube with the edge of length L in $\mathbf{R}^3$, i.e.,

$$\sigma_L = \{\pi^2 L^{-2} k^2,\ k \in \mathbf{Z}^3\} \tag{4}$$

The spectrum of an operator A will be denoted by $\sigma(A)$. If the operators Λ and Γ are defined in appropriate way (for instance, by means of corresponding quadratic forms), they will be self-adjoint and nonnegative, therefore their spectra lie on the positive semiaxis.

2.1. Band-Gap Structure of the Spectrum

Let us fix a positive L and introduce two parameters

$$b=\gamma(\delta L)^{-2}, \qquad w=\gamma\delta^{-3/2}L^{-2} \tag{5}$$

Then there exist an increasing function $a(\lambda)$: $[0, \infty)\mapsto[0, \infty)$ and a constant C such that for $N<Cb$ the following relationships hold:

$$\sigma(\Lambda)\cap[0, N]\subseteq \bigcup_{\mu\in\sigma_L, \mu\leqslant N}[\mu-a(N)\,w, \mu+a(N)\,w] \tag{6}$$

$$\sigma(\Lambda)\cap[\mu-a(N)\,w, \mu+a(N)\,w]\neq\varnothing, \qquad \mu\in\sigma_L\cap[0, N] \tag{7}$$

$$\sigma(\Gamma)\cap[0, N]\subseteq \bigcup_{\mu\in\sigma_L, \mu\leqslant N}[\mu-a(N)\,w, \mu+a(N)\,w] \tag{8}$$

$$\sigma(\Gamma)\cap[\mu-a(N)\,w, \mu+a(N)\,w]\neq\varnothing, \qquad \mu\in\sigma_L\cap[0, N] \tag{9}$$

In other words, for sufficiently small w the spectra of Λ and Γ in the interval $[0, N]$ lie in a vicinity (of width proportional to w) of σ_L, and each interval of this vicinity contains a nontrivial portion of the spectra $\sigma(\Lambda)$ and $\sigma(\Gamma)$ correspondingly.

This statement shows, in particular, that for sufficiently small values of parameters w and b^{-1} the spectra will be concentrated very close to the discrete set σ_L, so the spectral gaps do exist, and their location can be predicted.

2.2. Sketch of the Proof

Rescaling by $x'=x/L$, one can reduce the problem to the case when $L=1$, and so from now on we assume that $L=1$. Thus, ε is a 1-*periodic* function of $x\in\mathbf{R}^3$. The standard fundamental domain of periods is denoted by Q, i.e.,

$$Q=\{x\in\mathbf{R}^3: 0\leqslant x_j\leqslant 1, 1\leqslant j\leqslant 3\}$$

Since the operators Λ and Γ are periodic ones, we can apply the Bloch–Floquet theory[16–18] and decompose them into the direct integrals

$$\Lambda=\int_M^{\oplus}\Lambda(k)\,dk, \qquad \Gamma=\int_M^{\oplus}\Gamma(k)\,dk \tag{10}$$

where $M = 2\pi[0, 1]^3$ is the corresponding Brillouin zone, k is the quasimomentum, and the operators $\Lambda(k)$ and $\Gamma(k)$ can be described either as some differential operators on the cell Q with appropriate boundary conditions, or some differential operators on the torus $\mathbf{T}^3 = \mathbf{R}^3/\mathbf{Z}^3$.[16-18] The spectra of the operators Λ and Γ can be represented as follows:

$$\sigma(\Lambda) = \bigcup_{k \in M} \sigma(\Lambda(k)), \qquad \sigma(\Gamma) = \bigcup_{k \in M} \sigma(\Gamma(k)) \tag{11}$$

In order to find the spectra of the operators $\Lambda(k)$ and $\Gamma(k)$, we consider the eigenvalue problems

$$\Lambda(k)\, \Psi(x) = \lambda \Psi(x), \qquad \Gamma(k)\, \Psi(x) = \lambda \Psi(x) \tag{12}$$

We shall treat O here as a part of the torus $\mathbf{T}^3$ and introduce the region $T = \mathbf{T}^3 - O$. The common boundary of O and T is denoted by $\partial O = \partial T$, and Ψ_O and Ψ_T are, respectively, the restrictions of Ψ on O and T. Equations (12) can represented as follows:

Operator Λ:

$$\nabla_k \times (\nabla_k \times \Psi_O) = \lambda \Psi_O, \quad x \in O, \qquad \gamma \nabla_k \times (\nabla_k \times \Psi_T) = \lambda \Psi_T, \quad x \in T \tag{13}$$

$$\nabla_k \cdot \Psi_O = 0, \quad x \in O, \qquad \nabla_k \cdot \Psi_T = 0, \quad x \in T \tag{14}$$

$$\begin{gathered} \Psi_O|_{\partial O} = \Psi_T|_{\partial O} \\ \nu \times (\nabla_k \times \Psi_O)|_{\partial O} = \gamma \nu \times (\nabla_k \times \Psi_T)|_{\partial O} \\ \nu \cdot (\nabla_k \times \Psi_O)|_{\partial O} = \nu \cdot (\nabla_k \times \Psi_T)|_{\partial O} \end{gathered} \tag{15}$$

Operator Γ:

$$-\Delta_k \psi_O = \lambda \psi_O, \quad x \in O, \qquad -\gamma \Delta_k \psi_T = \lambda \psi_T, \quad x \in T \tag{16}$$

$$\psi_O|_{\partial O} = \psi_T|_{\partial O}, \qquad \nu \cdot \nabla_k \psi_O|_{\partial O} = \gamma \nu \cdot \nabla_k \psi_T|_{\partial O} \tag{17}$$

where ν is the normal vector to ∂O. Here we denote by ∇_k the operator $\nabla - ik$, where i is the imaginary unit, and by Δ_k the operator $(\nabla - ik)^2$. Equations (15) are the implementation of the well-known relationships for the tangent and normal components of the electromagnetic field E and the magnetic field H on discontinuity surfaces of dielectric constant ε or/and magnetic permittivity μ.

We shall consider now for simplicity the case $k = 0$ and Eqs. (16), (17). We can reduce the boundary problem (16), (17) on the cell Q to a boundary problem on just cube O as follows. Let us consider the Dirichlet problem on the set T,

$$-\gamma \Delta \psi_T = \lambda \psi_T, \quad x \in T, \qquad \psi_T(x)|_{\partial T} = \varphi(x), \quad x \in \partial O \tag{18}$$

where φ is a function on ∂O from an appropriate Sobolev space. We solve this problem and define the operator $K: \varphi \mapsto \nu \cdot \nabla\psi_T|_{\partial O}$. In other words, the operator K maps the Dirichlet boundary condition described by the function φ into the normal derivative of the solution of the Dirichlet boundary value problem on the boundary $\partial T = \partial O$ (K is called the Dirichlet-to-Neumann mapping). The operator K depends on γ and δ (in the case of an arbitrary $k \in M$ it depends also on k), i.e., $K = K_{\delta\gamma,\delta,k}$. Suppose now that ψ_O, ψ_T solve the problem (16), (17). Then we may treat the second equation in (16) and the first boundary equation (17) as the Dirichlet problem (18), where $\varphi = \psi_O(x)|_{\partial O}$. Then using the operator K we may rewrite the first equation in (16) and second boundary equation in (17) as follows:

$$-\nabla\psi_O = \lambda\psi_O, \quad x \in O, \qquad \nu \cdot \nabla\psi_O|_{\partial O} - \gamma K(\psi_O|_{\partial O}) = 0 \tag{19}$$

In other words, we may replace the original boundary value problem (16), (17) on the cell Q by the boundary value problem (19) on the cube O. Using parameters (5) we can rewrite the problem (19) as follows:

$$-\nabla\psi_O = \lambda\psi_O, \quad x \in O, \qquad \nu \cdot \nabla\psi_O|_{\partial O} - w[\delta^{3/2}K](\psi_O|_{\partial O}) = 0 \tag{20}$$

One can show that the norm of the operator $\delta^{3/2}K$ as an operator acting in appropriate Sobolev spaces of functions on the boundary ∂O has uniformly (with respect to all parameters) bounded norm, if w and b^{-1} are sufficiently small, and so *the problem* (20) *can be viewed as a perturbed Neumann boundary problem on the cube O*. This observation leads straightforwardly to the statements (8) and (9). The proof of the relationships (6) and (7) is analogous.

The fact that not only the operator $\delta^{3/2}K$, but even the operator δK is uniformly bounded can be easily seen for the one-dimensional analog of the problem (16), (17). Namely, in this case we consider the interval [0, 1], which we treat as a torus, and the analog of (16), (17) for $k = 0$ can be written as follows:

$$[0, 1] = T \cup O, \qquad T = [0, \delta], \quad O = [\delta, 1]$$

$$-\psi_O'' = \lambda\psi_O, \quad \delta \leqslant x \leqslant 1, \qquad -\gamma\psi_T'' = \lambda\psi_T, \quad 0 \leqslant x \leqslant \delta \tag{21}$$

$$\psi_O(\delta) = \psi_T(\delta), \quad \psi_O'(\delta) = \gamma\psi_T'(\delta), \qquad \psi_O(1) = \psi_T(0), \quad \psi_O'(1) = \gamma\psi_T'(0) \tag{22}$$

The analog of the Dirichlet problem in this case is

$$-\gamma\psi_T'' = \lambda\psi_T, \quad 0 \leqslant x \leqslant \delta, \qquad \psi_T(0) = \varphi(0), \qquad \psi_T(\delta) = \varphi(\delta) \tag{23}$$

and the operator K can be represented as follows:

$$K\begin{bmatrix}\varphi(0)\\ \varphi(\delta)\end{bmatrix}=(\lambda/\gamma)^{1/2}\,[\sin(\lambda/\gamma)^{1/2}\,\delta]^{-1}$$

$$\times\begin{bmatrix}-\cos(\lambda/\gamma)^{1/2}\,\delta & 1\\ -1 & \cos(\lambda/\gamma)^{1/2}\,\delta\end{bmatrix}\begin{bmatrix}\varphi(0)\\ \varphi(\delta)\end{bmatrix} \tag{24}$$

Therefore, if we take into account (5) and introduce a new parameter $w'=\gamma/\delta$, we can write the analog of the modified Neumann problem (20) in the following form:

$$-\psi_O''=\lambda\psi_O, \qquad \delta\leqslant x\leqslant 1 \tag{25}$$

$$\psi_O'(1)-w'\beta[\psi_O(\delta)-\cos(\lambda/b)^{1/2}\,\psi_O(1)]=0 \tag{26}$$

$$\psi_O'(\delta)-w'\beta[-\psi_O(1)+\cos(\lambda/b)^{1/2}\,\psi_O(\delta)]=0 \tag{27}$$

$$\beta=\delta(\lambda/\gamma)^{1/2}\,[\sin(\lambda/\gamma)^{1/2}\,\delta]^{-1}=(\lambda/b)^{1/2}\,[\sin(\lambda/b)^{1/2}]^{-1} \tag{28}$$

It is clear now that if b^{-1} and w' are sufficiently small, then β is close to 1, and the eigenvalues of the problem (25)–(28) lie in a vicinity proportional to w' of the spectrum of the corresponding Neumann problem [i.e., the problem (25)–(28) for $w'=0$]. In other words, the analogs of the formulas (8) and (9) hold.

Remark. One might wonder whether the condition that $\gamma/\delta^{3/2}$ is small is necessary, or the weaker condition of smallness of γ/δ (as in the one-dimensional case) is sufficient. Our proof requires so far $\gamma/\delta^{3/2}$, but this might be an artifact of the technique.

3. COMMENTS AND CONCLUSIONS

The qualitative picture of the behavior of the spectrum can be presented as follows. One may think of the spectrum σ of either operator Λ or Γ being close to the union of two spectra σ_T and σ_O, where σ_T is the spectrum of the Dirichlet problem with zero boundary conditions on the domain T (this part of the spectrum lies very high), and σ_O is the spectrum of the Neumann problem with zero normal derivative on the boundary of the domain O (for the one-dimensional model this can be verified by straightforward computation). This observation can be used to describe in simple fashion the mechanism of the rise of gaps in the spectrum σ and conditions under which this can happen. Remembering that we consider the high values for ε(or, equivalently, small γ), the following conclusions can be made.

1. The spectrum σ_T, being the spectrum of a relevant Dirichlet problem, has the minimum eigenvalue of the order b [for the one-dimensional model this can be seen from the expression (28) for β and boundary conditions (26)–(27)]. Thus, if we want to have a gap G of a fixed finite size centered at a given point we must keep b^{-1} sufficiently small (at least ought to be well above the center of G).

2. If b^{-1} tends to be small, then this together with the smallness of γ forces δ to be small, so the cube $O = O_\delta$ approaches the fixed unit cube Q, and the corresponding spectrum σ_O tends to be the spectrum σ_N of the Neumann problem on the cube S with zero normal derivative. So the limit location of the centers of the bands of the spectrum as γ, $b^{-1} \to 0$ coincides with the spectrum σ_N (this is proved also in ref. 15 in the sense of pseudogaps instead of gaps).

3. The width of the bands of the spectrum is of order w, as was explained before. Thus, to open up gaps, w ought to be small enough. In other words, both the width of the background "corridor" between the "air bubbles" and the inverse contrast ε^{-1} must tend to zero, but the rates of these asymptotics must be related (one with respect to another must be neither too fast nor too slow). The condition that w also tends to zero is not necessary for the existence of pseudogaps.[15]

4. The cubic form of the atom of embedded component is in a way optimal. The more general constraint on the atom of embedded material which provides the existence of gaps is the following. The shape of the atom (or combination of atoms which form a periodic cell) of the embedded material should be such that one can pack the space $\mathbf{R}^3$ by the atoms of this shape. Therefore, the ball-like atoms are not good in this regard, and the corresponding media exhibit pseudogaps rather than real gaps (the existence of such pseudogaps is proved in ref. 15).

The complete proofs of the results are rather lengthy, and they will be provided in subsequent articles. An analysis of the proofs shows that the function $a(N)$ and the constant C in the main statement can be estimated explicitly. We plan to provide explicit analytic and numerical estimates elsewhere.

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