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Existence of Gaps in the Spectrum of Periodic Dielectric Structures on a Lattice

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We consider the finite-difference counterpart, i.e., the true lattice analog, of Maxwell's equations and equations that govern the propagation of acoustic waves in a medium with a periodic dielectric structure. In particular, the vector nature of electromagnetic waves is fully taken into account. The existence of true gaps for these lattice models is proved for a two-component medium for which the dielectric constant is everywhere real and positive, and the dielectric constant of the background is essentially larger than the one corresponding to the embedded component.

KEY WORDS: Periodic dielectrics; Maxwell equations; lattice models; gaps in the spectrum.

INTRODUCTION

The problem of the existence of gaps for periodic dielectric structures associated with classical electromagnetic and acoustic waves has received considerable recent attention.[1-10] One of the important motivations for this type of problem is the intimate relationship of this problem to the problem of the Anderson localization of classical waves in a random medium.[1,2] The cited papers indicate that one can expect the rise of the gaps (or pseudogaps) in two-component dielectric structures under certain conditions on the background (host) and embedded components. Namely, the important parameters of the periodic medium which can shape the spectrum are the volume filling fraction, the dielectric constant ratio $\varepsilon_h/\varepsilon_e$ (where ε_h and ε_e are, respectively, the dielectric constants of the host material and the embedded components), and the shape of atoms of

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the embedded material as well as their arrangement. In particular, high dielectric constant ratio favors the rise of gaps in the spectrum.

In this paper the embedded component is assumed to consist of bounded atoms that do not overlap; therefore, the host material (or background) is a geometrically connected set. Such a dielectric medium can be rather easily fabricated in experiments (such as air domains in a dielectric background) and is quite promising in the context of the existence of a photonic gap.[6] Some types of living tissue (due to the cell structure which they naturally possess) can be examples of such a medium.[11] We consider the case when the host material is optically more dense, i.e., $\varepsilon_h \gg \varepsilon_e$. For the lattice version of Maxwell's equation (which fully takes into account the vector nature of electromagnetic waves) and for the medium described above we obtain the following results for sufficiently high dielectric constant ratio: (i) the spectrum has true gaps; (ii) in the case of acoustic waves, the centers of the permitted energy bands can be associated with a relevant Neumann-type boundary problem for the atoms of embedded material; (iii) the energy of wave modes associated with permitted bands of the spectrum resides for the most part in the atoms of the embedded component. The second statement shows how the single atom shapes the spectrum and, in particular, the gap structure for the medium discussed. The third statement indicates the importance of the wave nature of the scattering, since, from the geometrical optics point of view, because of the full reflection phenomenon, one might expect photons to reside in the more dense host material.

1. CONSTRUCTION OF LATTICE MODELS

To study the properties of wave propagation in a nonhomogeneous medium it is important to investigate the spectral properties of the relevant self-adjoint differential operators with coefficients varying in space. These operators for electromagnetic and acoustic waves have respectively the forms

$$\Lambda \Psi = \nabla \times [\gamma(x) \nabla \times \Psi], \qquad \gamma(x) = \varepsilon^{-1}(x)$$
$$\Gamma \psi = - \sum_{j=1}^{3} \frac{\partial}{\partial x_j} \gamma(x) \frac{\partial}{\partial x_j} \psi$$

In these formulas $\Psi(x)$ is a complex vector function, $\psi(x)$ is a complex scalar function, and $\varepsilon(x)$ stands for the electric permitivity for electromagnetic waves, whereas for acoustic waves $\varepsilon^{-1}(x)$ stands for the coefficient of elasticity of the medium. We suppose the coefficient $\varepsilon(x)$, $x \in \mathbb{R}^3$, to be a periodic field bounded from above and below by positive constants.

In the case of a random field, according to the philosophy of the propagation of waves in a random medium[12] (Anderson localization[13]), we may expect the rise of localized states, i.e., the rise of the purely point spectrum, under some conditions. In particular, as has been pointed out,[1,2,12] the problem of the existence of localized states for random media is connected with the problem of the existence of gaps in the spectrum for periodic media as follows. Suppose $\varepsilon_0(x)$ is a positive periodic field and $\varepsilon(x) = \varepsilon_0(x) + \varepsilon_1(x)$, where $\varepsilon_1(x)$ is a small random field. If the spectrum of the operator associated with periodic $\varepsilon_0(x)$ has gaps, the the operator associated with $\varepsilon(x)$ can develop localized states in those gaps. In particular, this mechanism can work for electromagnetic or acoustic waves.[1,2] Thus it is important to know whether there are gaps in the relevant spectrum. In spite of a similarity between the second-order operators Λ and Γ on one hand and the Schrödinger operator on other, there is an important difference that makes it difficult to construct a disordered medium which can have localized states. In particular, the difference is that for operators Λ and Γ the bottom of the spectrum does not depend on the coefficient $\varepsilon(x)$ at all and equals zero, whereas for the Schrödinger operator it depends on the potential and this is why localized states might appear in a vicinity of the bottom of the spectrum. That is, in order to apply the above philosophy we have to construct first a medium (for instance, a periodic one) possessing a true gap in the spectrum.[1,2] In this paper we prove the existence of gaps for the lattice analogs of the operators Λ and Γ which are constructed below.

We begin with a construction of the discrete analogs of the operators Λ and Γ keeping the same notation for them. We construct the lattice version of the operators of interest in a way similar to the Anderson tight-binding model,[13] replacing the differential operators by their finite-difference counterparts. Namely, we introduce discrete analogs of the partial derivatives ∂_j and ∇ as follows. Let V_j, $1 \leqslant j \leqslant d$ (d is the dimension of the space, i.e., 3 in many interesting cases), be the unitary shift operators acting on Hilbert space $l_2(\mathbb{Z}^d)$ or $l_2^n(\mathbb{Z}^d)$ [that is, the direct sum of n copies of $l_2(\mathbb{Z}^d)$, where n stands for the dimension of the vectors; n equals 3 for electromagnetic waves and 1 for acoustic waves]. If e_j, $1 \leqslant j \leqslant d$, are the standard basis vectors in lattice $\mathbb{Z}^d$ and I is the identity operator, then V_j and ∂_j are defined by

$$\begin{aligned} (V_j \Psi)(m) &= \Psi(S_j(m)), \qquad S_j(m) = m - e_j, \quad m \in \mathbb{Z}^d \\ \partial_j &= I - V_j, \qquad 1 \leqslant j \leqslant d \end{aligned} \tag{1.1}$$

That is, S_j stands for the shift in lattice $\mathbb{Z}^d$ by the vector e_j. The discrete analog of ∇ we define by substituting the partial derivatives by their counterparts ∂_j from (1.1). We can incorporate both the electromagnetic and acoustic cases as follows.

Let us first introduce operators on the lattice which are the analogs of differential operators. We denote by $f_{m,r}$, $m \in \mathbb{Z}^d$, $1 \leqslant r \leqslant n$, the standard orthonormal basis in $l_2^n(\mathbb{Z}^d)$, i.e., $(f_{m,r})(k, q) = \delta_{m,k}\delta_{r,q}$, $m, k \in \mathbb{Z}^d$, $1 \leqslant r$, $q \leqslant n$, where δ is the Kronecker delta symbol. In view of (1.1) we obviously have

$$V_j^{-1} f_{m,r} = f_{m-e_j,r}, \qquad m \in \mathbb{Z}^d, \quad 1 \leqslant r \leqslant n, \quad 1 \leqslant j \leqslant d$$

$$(V_j^{-1}\Psi)(m, r) = \Psi(m + e_j, r), \qquad m \in \mathbb{Z}^d, \quad 1 \leqslant r \leqslant n, \quad 1 \leqslant j \leqslant d$$

Definition. Let us call a linear operator D acting in the Hilbert space $l_2^n(\mathbb{Z}^d)$ a ∂-operator if for some complex constants $d_{r,q;j}$, $1 \leqslant r, q \leqslant n$, $1 \leqslant j \leqslant d$, the following representation is valid:

$$(D\Psi)(m, r) = \sum_{q=1}^{n} \sum_{j=1}^{d} d_{r,q;j} (\partial_j \Psi)(m, q) \tag{1.2}$$

where ∂_j are defined by (1.1), that is, $(\partial_j \Psi)(m, q) = \Psi(m, q) - \Psi(m - e_j, q)$, $m \in \mathbb{Z}^d$.

In particular, it is obvious that discrete ∂_j are ∂-operators, and the discrete curl operator $\nabla \times (\cdot)$ is a ∂-operator as well for $d = n = 3$ and matrices $\{d_{r,q;j}\}$ defined by

$$\{d_{r,q;1}\} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \qquad \{d_{r,q;2}\} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$$
$$\{d_{r,q;3}\} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{1.3}$$

We next define quadratic forms that will be associated with the desired self-adjoint operators. Namely if D_l, $1 \leqslant l \leqslant N$, are ∂-operators in $l_2^n(\mathbb{Z}^d)$, then

$$Q(\Psi, \Psi) = \sum_{m \in \mathbb{Z}^d} \gamma(m) \sum_{l=1}^{N} |(D_l \Psi)_m|^2$$

We associate with this form Q the self-adjoint operator

$$A = \sum_{l=1}^{N} D_l^* \gamma D_l$$

In particular,

$$A = \Lambda \qquad \text{if} \quad N = 1, \quad d = n = 3, \quad D_1(\cdot) = \nabla \times (\cdot) \tag{1.4}$$

$$A = \Gamma \qquad \text{if} \quad N = d, \quad n = 1, \quad D_l = \partial_l, \quad 1 \leqslant l \leqslant d \tag{1.5}$$

Two-Component Medium

To establish accurate results we must specify the medium, i.e., the function $\varepsilon(m)$, $m \in \mathbb{Z}^d$. We consider a two-component medium, that is, a medium for which the function ε takes on just two values, 1 and $\xi > 1$. In fact, we will be especially interested in $\xi \gg 1$. Thus, one may think of the two-component medium as a set of connected domains (atoms) where $\varepsilon = 1$ which are embedded into a medium with higher $\varepsilon = \xi$. Now consider the set $\mathscr{A}$ of the sites of the lattice where ε takes on the value 1, and set $\mathscr{F} = \mathbb{Z}^d/\mathscr{A}$, where ε takes on the value ξ, i.e.,

$$\gamma(m) = \varepsilon^{-1}(m) = \begin{cases} 1 & \text{if} \quad m \in \mathscr{A} \\ \xi^{-1} & \text{if} \quad m \in \mathscr{F} \end{cases} \tag{1.6}$$

Definition. We say that two sites m and m' are neighboring if there is $j \in \{1,..., d\}$ such that $m - m' = \pm e_j$. A subset $\mathscr{A}$ of the lattice is called connected if for any two elements x and y there is a finite sequence $x_1,..., x_l$ such that $x_q \in \mathscr{A}$, $1 \leqslant q \leqslant l$, $x_1 = x$, $x_l = y$, and each pair of elements x_q, x_{q+1}, $1 \leqslant q \leqslant l - 1$, are neighboring.

We can decompose the set $\mathscr{A}$ into the union of its connected components $\mathscr{A}_\alpha$, namely

$$\mathscr{A} = \bigcup_{\alpha \in Z} \mathscr{A}_\alpha, \qquad \mathscr{A}_\alpha \cap \mathscr{A}_\beta = \varnothing \qquad \text{if} \quad \alpha \neq \beta \tag{1.7}$$

where Z is a set of indexes (it might be the set of natural numbers or, for instance, the lattice $\mathbb{Z}^d$, if we want to build a periodic structure). For the sake of simplicity in the spectral analysis of the operators associated with the sets $\mathscr{A}_\alpha$, we pose some constraints on these sets.

Assumption C. All connected subsets $\mathscr{A}_\alpha$ in the decomposition (1.7) are finite and for any two different $\mathscr{A}_\alpha$ and $\mathscr{A}_\beta$ if $x \in \mathscr{A}_\alpha$ and $y \in \mathscr{A}_\beta$, then x and y are not neighboring or equal and there is no site z neighboring both x and y.

Assumption C means that the connected components $\mathscr{A}_\alpha$ cannot be too close to each other. Let us consider a simple but important example when the subsets $\mathscr{A}_\alpha$ are parallelepipeds. Namely, let $p_1, ..., p_d$ be natural integers and

$$\mathscr{A}_0 = \{0,..., p_1 - 1\} \times \cdots \times \{0,..., p_d - 1\}$$

$$\mathscr{A} = \bigcup_{\alpha \in \mathbb{Z}^d} \mathscr{A}_\alpha, \qquad \alpha = (\alpha_1,..., \alpha_d)$$

$$\mathscr{A}_\alpha = \mathscr{A}_0 + (\alpha_1 r_1,..., \alpha_d r_d), \qquad r_j \geqslant p_j + 2, \quad 1 \leqslant j \leqslant d$$

In this case the sets $\mathscr{A}_\alpha$ are obviously connected and, because of the inequalities for r_j, it is not difficult to verify that they satisfy Assumption C.

Now if D_l, $1 \leqslant l \leqslant N$, are ∂-operators, then we have the following quadratic form associated with the function ε defined by (1.6):

$$Q(\Psi, \Psi) = \xi^{-1} Q_{\mathscr{F}}(\Psi, \Psi) + \sum_{\alpha \in Z} Q_{\mathscr{A}_\alpha}(\Psi, \Psi) \tag{1.8}$$

$$Q_{\mathscr{B}}(\Psi, \Psi) = \sum_{m \in \mathscr{B}} \sum_{l=1}^{N} |(D_l \Psi)_m|^2, \qquad \mathscr{B} \subseteq \mathbb{Z}^d \tag{1.9}$$

That is, the quadratic forms $Q_{\mathscr{A}_\alpha}$ are associated with the portion of the lattice where ε is 1, whereas $Q_{\mathscr{F}}$ is associated with the rest of the lattice where ε equals ξ. The self-adjoint operator associated with the quadratic form (1.8) is

$$\mathfrak{A} = \sum_{l=1}^{N} D_l^* \gamma D_l, \qquad \text{where } \varepsilon \text{ is defined by (1.6)} \tag{1.10}$$

2. STATEMENT OF RESULTS

We suppose here that the operator $\mathfrak{A}$ is defined by (1.10), where D_l are ∂-operators defined by (1.2). Since we are interested in the operators $\mathfrak{A}$ for large ξ, let us first consider the operator $\mathfrak{A}^{(0)} = \mathfrak{A}|_{\xi = \infty}$. This self-adjoint operator is associated with the second sum in (1.8) and can be represented as follows:

$$\mathfrak{A}^{(0)} = \mathfrak{A}_{\mathscr{A}} = \sum_{\alpha \in Z} \mathfrak{A}_{\mathscr{A}_\alpha} \tag{2.1}$$

where for any $\mathscr{B} \subseteq \mathbb{Z}^d$

$$\mathfrak{A}_{\mathscr{B}} = \sum_{l=1}^{N} D_l^* \chi_{\mathscr{B}} D_l, \qquad \chi_{\mathscr{B}}(m) = \begin{cases} 1 & \text{if } m \in \mathscr{B} \\ 0 & \text{if } m \notin \mathscr{F} \end{cases} \tag{2.2}$$

Now we have the following representation for the operator $\mathfrak{A}$:

$$\mathfrak{A} = \xi^{-1}\mathfrak{A}_{\mathscr{F}} + \mathfrak{A}_{\mathscr{A}} = \xi^{-1}\mathfrak{A}_{\mathscr{F}} + \mathfrak{A}^{(0)} = \xi^{-1}\mathfrak{A}_{\mathscr{F}} + \sum_{\alpha \in Z} \mathfrak{A}_{\mathscr{A}_\alpha} \tag{2.3}$$

First of all we notice that all operators $\mathfrak{A}$, $\mathfrak{A}^{(0)}$, and $\mathfrak{A}_{\mathscr{B}}$ are obviously nonnegative and zero belongs to their spectra, i.e., if $\sigma(\mathfrak{C})$ stands for the spectrum of the operator $\mathfrak{C}$, then

$$\sigma(\mathfrak{A}),\ \sigma(\mathfrak{A}^{(0)}),\ \sigma(\mathfrak{A}_{\mathscr{B}}) \ni 0 \tag{2.4}$$

Theorem 1 (Spectrum for $\xi = \infty$). Suppose that Assumption C is satisfied. Then $\mathfrak{A}_{\mathscr{A}_\alpha}\mathfrak{A}_{\mathscr{A}_\beta} = 0$ if $\alpha \neq \beta$ and therefore the sum of operators in (2.1) is direct, and

$$\sigma(\mathfrak{A}^{(0)}) = \bigcup_{\alpha \in Z} \sigma(\mathfrak{A}_{\mathscr{A}_\alpha}) \tag{2.5}$$

If in addition the sets $\mathscr{A}_\alpha$ form a periodic structure, that is, there is a vector $r = (r_1,..., r_d) \in \mathbb{Z}^d$ with positive components (big enough to satisfy Assumption C), such that $\mathscr{A}_\alpha = \mathscr{A}_0 + (\alpha_1 r_1,..., \alpha_d r_d)$ where $\mathscr{A}_0$ is a nonempty finite set, then

$$\sigma(\mathfrak{A}^{(0)}) = \sigma(\mathfrak{A}_{\mathscr{A}_0}) \tag{2.6}$$

where $\sigma(\mathfrak{A}_{\mathscr{A}_0})$ is a finite set containing at least two distinct points one of which is 0.

Thus Theorem 1 states that the spectrum of operator $\mathfrak{A}^{(0)}$ is a discrete set. In particular, the spectrum is a finite set in the case of a periodic medium (in this case, of course, the eigenvalues have an infinite multiplicity). Let us suppose for a moment that the medium is periodic and therefore the operator $\mathfrak{A}$ has only an absolutely continuous spectrum which is a set of intervals in the real axis. In this case if ξ is large eneough, the operator $\mathfrak{A}$, being a small perturbation of the operator $\mathfrak{A}^{(0)}$, must have gaps in the spectrum, since the spectrum $\sigma(\mathfrak{A})$ has to be in the vicinity of the appropriate finite set $\sigma(\mathfrak{A}_{\mathscr{A}_0})$. Let us define accurately what we mean by a gap in the spectrum.

Definition (Gap). We say that a self-adjoint operator A has a gap in its spectrum if there are finite real numbers $\lambda_1 < \lambda_2$ such that $\lambda_1, \lambda_2 \in \sigma(A)$, $(\lambda_1, \lambda_2) \cap \sigma(A) = \varnothing$. That is, there are points of the spectrum to the right and to the left of the gap.

Theorem 2 (Existence of gaps). Suppose that Assumption C is satisfied and the medium is periodic as defined in the statement of Theorem 1. Then if ξ is large enough, the spectrum of the operator $\mathfrak{A}$ has gaps and moreover it is located in the vicinity of the finite set $\sigma(\mathfrak{A}_{\mathscr{A}_0})$. Specifically, the spectrum of the operator $\mathfrak{A}$ has a gap if the following inequality is satisfied:

$$\xi\lambda_1(\mathfrak{A}_{\mathscr{A}_0}) > 8d \sum_{l=1}^{N} \sum_{j=1}^{d} \|\{d_j^{(l)}\}\|^2 \tag{2.7}$$

where $\lambda_1(\mathfrak{A}_{\mathscr{A}_0})$ is the smallest positive eigenvalue associated with the matrix $\mathfrak{A}_{\mathscr{A}_0}$. In particular, if $\mathscr{A}_0 = \{0,..., p_1 - 1\} \times \cdots \times \{0,..., p_d - 1\}$ is a parallelepiped, then in the cases of the operators Λ and Γ the following inequalities guarantee the existence of a gap in the spectrum

$$\Lambda\colon \quad \xi\lambda_1(\Lambda_{\mathscr{A}_0}) > 48 \tag{2.8}$$

$$\Gamma\colon \quad \xi > 8d(d+1)\sin^{-2}\frac{\pi}{p(\mathscr{A}_0)}, \qquad p(\mathscr{A}_0) = \max_{1 \leqslant j \leqslant d} p_j \tag{2.9}$$

By the way, the last inequality is obtained on the base of a sort of Neumann boundary problem. More generally, we first notice that $(\Psi, \mathfrak{A}_{\mathscr{B}}\Psi) = Q_{\mathscr{B}}(\Psi, \Psi)$, where the quadratic form $Q_{\mathscr{B}}$ defined by (1.9). Then, in view of this representation and the fact that $Q_{\mathscr{B}}$ is defined for all Ψ in the Hilbert space, we may think of the operator $\mathfrak{A}_{\mathscr{B}}$ as an operator associated with a sort of Neumann boundary problem (see also Lemma 2 and comments in its proof).

Remark. For the considered lattice models of periodic dielectric structures we can list the following factors that shape the spectrum and, in particular, gaps: (i) the connectedness of the host component and the atomic structure of the embedded component (the filling fraction of the embedded material might have an impact on the smallest dielectric constant ratio under which a gap in the spectrum rises); (ii) the atoms of the embedded material shape the band structure of the spectrum.

3. PROOF OF RESULTS

We suppose here that Assumption C is satisfied. For $\mathscr{B} \subseteq \mathbb{Z}^d$, let $H_{\mathscr{B}}$ be the Hilbert subspace of $l_2^n(\mathbb{Z}^d)$ made up of vectors Ψ such that $\Psi(m) = 0$ if $m \notin \mathscr{B}$. In addition, for any $\mathscr{B} \subseteq \mathbb{Z}^d$ we introduce its extension

$$\mathscr{B}' = \mathscr{B} \bigcup_{j=1}^{d} S_j\mathscr{B} \tag{3.1}$$

where the shift operators S_j are defined in (1.1). In other words, the set $\mathscr{B}'$ can be obtained from $\mathscr{B}$ by joining to it a part of the neighboring sites of the lattice.

Lemma 1. The following statements are true

(i) For any $\mathscr{B} \in \mathbb{Z}^d$: $\mathfrak{A}_{\mathscr{B}} H_{\mathscr{B}'}^{\perp} = 0$, $\mathfrak{A}_{\mathscr{B}} H_{\mathscr{B}'} \subseteq H_{\mathscr{B}'}$

(ii) $\mathscr{A}'_\alpha \cap \mathscr{A}'_\beta = \varnothing$ and $\mathfrak{A}_{\mathscr{A}_\alpha} \mathfrak{A}_{\mathscr{A}_\beta} = 0$ if $\alpha \neq \beta$, and therefore the sum of operators in (2.1) is direct.

(iii) If $\mathscr{B}$ is a finite and connected subset of the lattice, then there is an eigenvector Ψ, namely $\Psi(m) \equiv 1$, $m \in \mathscr{B}$, such that $\mathfrak{A}_{\mathscr{B}} \Psi = 0$. If $\mathfrak{A} = \Gamma$, then Ψ is only an eigenvector such that $\Gamma_{\mathscr{B}} \Psi = 0$. If $\mathscr{B}$ is an infinite and connected subset of the lattice, then $\Gamma_{\mathscr{B}} \Psi = 0$ implies $\Psi = 0$.

(iv) Operators $\mathfrak{A}$, $\mathfrak{A}^{(0)}$, and $\mathfrak{A}_{\mathscr{B}}$ (for a finite and connected $\mathscr{B}$) are nonnegative and their spectra contain 0, that is, (2.4) is true.

Proof. Suppose that $x \in \mathscr{B}'^c$, where for a set $\mathscr{A}$, $\mathscr{A}^c$ is its complementary set. Since obviously $H_{\mathscr{B}'}^{\perp} = H_{\mathscr{B}'^c}$, then in order to verify the first statement in (*i*) it is sufficient to check that $\mathfrak{A}_{\mathscr{B}} f_x = 0$. Now, we notice that it follows from (1.2) that Df_x is a linear combination of the vector f_y, $y \in \{x + e_j,\ j = 1,..., d\}$. By the assumption made, $x \notin \mathscr{B}'$. Therefore $y = x + e_j \notin \mathscr{B}$, $j = 1,..., d$, and $\chi_{\mathscr{B}} f_x = 0$. That is, we have $\chi_{\mathscr{B}} Df_x = 0$. From this and (1.10) we obtain $\mathfrak{A}_{\mathscr{B}} f_x = 0$, which proves the first relationship in (i). The second relationship follows straightforwardly from first since $\mathfrak{A}_{\mathscr{B}}$ is obviously a self-adjoint operator.

Suppose now for a moment that there are α and β such that $\alpha \neq \beta$ and $\mathscr{A}'_\alpha \cap \mathscr{A}'_\beta \neq \varnothing$. Then from this we have to conclude that either there is j (or k) such that $x + e_j = y$ (or $x = y + e_k$) or there is a z such that $z = x + e_j = y + e_k$, where $x \in \mathscr{A}_\alpha$ and $y \in \mathscr{A}_\beta$ for some j and k. But all these contradict Assumption C. Hence the first relationship in (ii) is true. The second relationship follows easily from the first one and the statement (i).

The statement (iii) follows immediately from (1.9) and (2.2). The statement (iv) for $\mathfrak{A}_{\mathscr{B}}$ (for a finite and connected $\mathscr{B}$) obviously follows from the statement (iii). The statement (iv) for $\mathfrak{A}^{(0)}$ in turn follows from this statement for $\mathfrak{A}_{\mathscr{B}}$. As far as the operator $\mathfrak{A}$ is concerned, we can easily show that there is a sequence of vectors Ψ_n. $n = 1, 2,...,$ such that $\|\Psi_n\| = 1$ and $\lim_{n \to \infty} \|\mathfrak{A} \Psi_n\| = 0$. Namely, let us set $\Psi_n(m) = (2n)^{-d/2}$ if $m = (m_1,..., m_d)$, $|m_j| \leqslant n$, $1 \leqslant j \leqslant d$, and $\Psi_n(m) = 0$ otherwise. Straightforward computation shows that $\|\mathfrak{A} \Psi_n\|$ goes to zero as n approaches infinity at the rate n^{-1}. This completes the proof of the lemma. ∎

Proof of Theorem 1. The validity of the direct sum decomposition (2.1) for the operator $\mathfrak{A}^{(0)}$ follows immediately from Lemma 1(ii). The relationship (2.5) obviously follows from (2.1). As far as representation (2.6) is concerned, due to the supposed periodicity we obviously have

$$\mathfrak{A}_{\mathscr{A}_\alpha} = V^{-\alpha r}\mathfrak{A}_{\mathscr{A}_0} V^{\alpha r}, \qquad V^{\alpha r} = V_1^{\alpha_1 r_1} \cdots V_d^{\alpha_d r_d}, \qquad \sigma(\mathfrak{A}_{\mathscr{A}_\alpha}) = \sigma(\mathfrak{A}_{\mathscr{A}_0})$$

This relationships and (2.5) imply the validity of (2.6), which completes the proof of the theorem. ∎

Considering the gaps in the spectrum of the operators $\mathfrak{A}$, we will especially be interested in the first (or the lowest) gap. So, since in view of Lemma 1, the operators $\mathfrak{A}_{\mathscr{B}}$ are positive and their spectra contain 0, it would be useful to evaluate the first positive eigenvalue of $\mathfrak{A}_{\mathscr{B}}$, denoted by $\lambda_1(\mathfrak{A}_{\mathscr{B}})$.

Lemma 2. Suppose that $\mathfrak{A} = \Gamma$. If $\mathscr{P}$ is a parallelepiped on the lattice (i.e., $\mathscr{P} = \{0,..., p_1 - 1\} \times \cdots \times \{0,..., p_d - 1\}$, where p_j, $1 \leqslant j \leqslant d$, are natural numbers) and $p(\mathscr{P}) = \max_{1 \leqslant j \leqslant d} p_j$, then the following estimation is true:

$$\lambda_1(\Gamma_{\mathscr{P}}) \geqslant \lambda_{\mathscr{P}} = \frac{d}{d+1} \sin^2 \frac{\pi}{p(\mathscr{P})} \tag{3.2}$$

We may think of the matrix $\Gamma_{\mathscr{P}}$ as the one associated with a sort of Neumann boundary problem by the following reasons. First, in view of Lemma 1(iii), (iv), $\Gamma_{\mathscr{P}}$ is nonnegative and has a unique vector $\Psi(m) \equiv 1$ such that $\Gamma_{\mathscr{P}} \Psi = 0$. Second, the estimation (3.2) for the first nonnegative eigenvalue $\lambda_1(\Gamma_{\mathscr{P}})$ up to a factor is the same as for the relevant eigenvalue of a matrix $\mathfrak{B}_{\mathscr{P}}$ (constructed below) that can be associated Neumann boundary conditions.

To prove this lemma we need first to prove some auxiliary statements. Let $\mathscr{P}$ be a parallelepiped and let $\mathfrak{B}_{\mathscr{P}}$ be the quadratic form defined by

$$\mathfrak{B}_{\mathscr{P}}(\psi, \psi) = \sum_{\langle m,k \rangle \in \tilde{\mathscr{P}}} |\psi(m) - \psi(k)|^2 \tag{3.3}$$

where $\tilde{\mathscr{P}}$ is the set of all neighboring pairs $\langle m, k \rangle$ in $\mathscr{P}$. If $B_{\mathscr{P}}$ is a symmetric matrix associated with the form $\mathfrak{A}_{\mathscr{P}}$ then it is easy to see that its entries $B_{\mathscr{P}}(m, k)$ are equal to

$$B_{\mathscr{P}}(m, k) = \begin{cases} \nu(k) & \text{if } \ m = k \in \mathscr{P} \\ -1 & \text{if } \ \langle m, k \rangle \in \mathscr{P}' \\ 0 & \text{otherwise} \end{cases}$$

where $\nu(k)$ is the number of sites of the lattice in $\mathscr{P}$ neighboring site k.

By the way, one can easily verify that matrix $B_{\mathscr{P}}$ can be obtained from the following Neumann boundary problem. Let b be a point on the boundary $\partial\mathscr{P}$ of the parallelepiped $\mathscr{P}$ and $\mathscr{N}_b = \{b' : b' \notin \mathscr{P},\ b' \text{ is neighboring } b\}$. Thus matrix $B_{\mathscr{P}}$ can be obtained from matrix Γ provided by the following boundary conditions:

$$\psi(b) - \psi(b') = 0, \qquad b \in \partial\mathscr{P}, \qquad b' \in \mathscr{N}_b$$

Now if we define the set of vectors e_t as

$$e_t(k) = \prod_{j=1}^{d} \cos[\pi(2k_j + 1)\, t_j p_j^{-1}], \qquad t = (t_1, \ldots, t_d), \quad k = (k_1, \ldots, k_d) \in \mathscr{P}$$

then we can verify straightforwardly that they form a set of eigenvectors and

$$B_{\mathscr{P}} e_t = 2 \sum_{j=1}^{d} [1 - \cos(2\pi t_j p_j^{-1})]\, e_t, \qquad t \in \mathscr{P} \tag{3.4}$$

Lemma 3. Let $\mathfrak{B}_{\mathscr{P}}$ be a quadratic form defined by (3.3) for a parallelepiped $\mathscr{P}$ and $p(\mathscr{P}) = \max_{1 \leqslant j \leqslant d} p_j$. Then if $\lambda_1(\mathfrak{B}_{\mathscr{P}})$ is a minimal positive eigenvalue of $\mathfrak{B}_{\mathscr{P}}$, the following estimation is true:

$$\lambda_1(\mathfrak{B}_{\mathscr{P}}) \geqslant 2 \sin^2 \frac{\pi}{p(\mathscr{P})} \tag{3.5}$$

Proof. The inequality follows straightforwardly from (3.4). ∎

Proof of Lemma 2. Let us notice that for a parallelepiped $\mathscr{P}$ introduced above, the set $\mathscr{P}'$ defined by (3.1) can be decomposed as follows:

$$\mathscr{P} = \mathscr{P} \cup \left(\bigcup_{1 \leqslant j \leqslant d} \mathscr{P}_j \right)$$

where

$$\mathscr{P}_j = \{(k_1, \ldots, k_d) \in \mathbb{Z}^d : k_j = -1;\ 0 \leqslant k_q \leqslant p_q - 1,\ 1 \leqslant q \leqslant d,\ q \neq j\}, \qquad 1 \leqslant j \leqslant d$$

$$\mathscr{P} \cap \mathscr{P}_j = \varnothing, \qquad \mathscr{P}_j \cap \mathscr{P}_q = \varnothing, \qquad 1 \leqslant j, q \leqslant d, \qquad j \neq q$$

From this (2.2) and (3.3) we have

$$Q_{\mathscr{P}}(\psi, \psi) = (\psi, \Gamma_{\mathscr{P}} \psi) = \mathfrak{B}_{\mathscr{P}}(\psi, \psi) + \sum_{j=1}^{d} \sum_{l \in \mathscr{P}_j} |\psi(l) - \psi(l + e_j)|^2 \tag{3.6}$$

Since $\psi(m) \equiv 1$, $m \in \mathscr{P}$, is obviously the only vector on which the forms $\mathfrak{B}_{\mathscr{P}}$ and $Q_{\mathscr{P}}$ take on zero value [see Lemma 1(iii) and (3.3)], then in order to prove the lemma, it is sufficient to show that for any vector $\psi(m)$, $m \in \mathscr{P}$, the following inequality is true:

$$Q_{\mathscr{P}}(\psi, \psi) \geqslant \lambda_{\mathscr{P}} \sum_{m \in \mathscr{P}'} |\psi(m) - \psi_{\mathscr{P}'}|^2, \qquad \psi_{\mathscr{P}'} = N(\mathscr{P}')^{-1} \sum_{m \in \mathscr{P}'} \psi(m) \tag{3.7}$$

where $N(\mathscr{P}') = (p_1 + 1) \cdots (p_d + 1) - 1$ is the number of sites in the set $\mathscr{P}'$. In view of the remark above concerning the uniqueness of the vector on which the form $\mathfrak{B}_{\mathscr{P}}$ equals zero and (3.5), we have

$$\mathfrak{B}_{\mathscr{P}}(\psi, \psi) \geqslant \lambda_1(\mathfrak{B}_{\mathscr{P}}) \sum_{m \in \mathscr{P}} |\psi(m) - \psi_{\mathscr{P}}|^2, \qquad \psi_{\mathscr{P}} = N(\mathscr{P})^{-1} \sum_{m \in \mathscr{P}} \psi(m) \tag{3.8}$$

where $N(\mathscr{P}) = p_1 \cdots p_d$ is the number of sites in the parallelepiped $\mathscr{P}$. Hence from (3.6) and (3.8) we obtain

$$(\psi, \Gamma_{\mathscr{P}}) \geqslant \eta \sum_{m \in \mathscr{P}} |\varphi(m)|^2 + \sum_{j=1}^{d} \sum_{l \in \mathscr{P}_j} |\varphi(l) - \varphi(l + e_j)|^2, \qquad \eta = \lambda_1(\mathfrak{B}_{\mathscr{P}}) \tag{3.9}$$

where

$$\varphi(m) = \psi(m) - \psi_{\mathscr{P}}, \qquad \eta = \lambda_1(\mathfrak{B}_{\mathscr{P}}) \tag{3.10}$$

In order to estimate the right side of the last inequality we will need the following elementary inequality:

$$a|x|^2 + b|x - y|^2 \geqslant \{2[a^{-1} + (2b)^{-1}]\}^{-1}(|x|^2 + |y|)^2 \tag{3.11}$$

which is true for any positive a, b and complex x and y. Now we notice that the indices $l + e_j$ in the second sum in (3.9) belong to $\mathscr{P}$. Besides, the "left" boundary elements b from $\mathscr{P}$ (i.e., such $b \in \mathscr{P}$ that for a $j \in \{1,..., d\}$: $S_j b \notin \mathscr{P}$) can be represented in the form $b = l + e_j$, $l \in \mathscr{P}_j$, in several ways (for different j), but obviously not greater than in d ways. Now if we separate the summands from the first sum in (3.9) associated with the mentioned boundary elements b and join them to the second sum in (3.9) and then apply the inequality (3.11), $a = \eta d^{-1}$, $b = 1$ (taking in account the remark on the maximum number of possible representation of b), then we get the following estimate

$$(\psi, \Gamma_{\mathscr{P}} \psi) \geqslant d\eta(2d + \eta)^{-1} \sum_{m \in \mathscr{P}'} |\varphi(m)|^2 \tag{3.12}$$

Let us notice that

$$\min_{t \in \mathbb{C}} \sum_{m \in \mathscr{P}'} |\psi(m) - t|^2 = \sum_{m \in \mathscr{P}'} |\psi(m) - \psi_{\mathscr{P}'}|^2 \tag{3.13}$$

Now from (3.10), (3.5), (3.12), and (3.13) we can conclude that (3.7) is true and therefore (3.2) is true, which completes the proof of Lemma 2. ▮

Having in mind the representation (2.3), we need to evaluate the following norms.

Lemma 4. Let operators ∂_j, D, Λ, and Γ be defined correspondingly by (1.1), (1.2), (1.4), and (1.5), where $\gamma \equiv 1$. Then the following estimations of their norm are true:

$$\|\partial_j\| \leqslant 2, \qquad \|D\| \leqslant 2\left(d \sum_{j=1}^{d} \|\{d_j\}\|^2\right)^{1/2} \tag{3.14}$$

where $\|\{d\}_j\|$ is the norm of the matrix $\{d_{r,q;j}\}$, $1 \leqslant j \leqslant d$,

$$\|\Lambda\| \leqslant 24, \qquad \|\Gamma\| \leqslant 4d \tag{3.15}$$

Proof. The first inequality in (3.14) follows straightforwardly from (1.1). To prove the second one we note that

$$\begin{aligned}\sum_{r=1}^{n} |(D\Psi)(m, r)|^2 &= \sum_{r=1}^{n} \left| \sum_{q=1}^{n} \sum_{j=1}^{d} d_{r,q;j} (\partial_j \Psi)(m, q)\right|^2 \\ &= \left\| \sum_{j=1}^{d} \{d_j\} (\partial_j \Psi)(m) \right\|^2 \\ &\leqslant \left(\sum_{j=1}^{d} \|\{d_j\}\|^2\right) \sum_{j=1}^{d} \|(\partial_j \Psi)(m)\|^2\end{aligned}$$

Summing up both sides of the last inequality over $m \in \mathbb{Z}^d$ and using the inequality (3.14) for ∂_j, we easily obtain

$$\|D\Psi\|^2 \leqslant \left(\sum_{j=1}^{d} \|\{d_j\}\|^2\right) \sum_{j=1}^{d} \|(\partial_j \Psi)\|^2 \leqslant \left(4d \sum_{j=1}^{d} \|\{d_j\}\|^2\right) \|\Psi\|^2$$

For the operator Λ [see (1.3) and (1.4)] we have $N = 1$, $n = d = 3$, and $\|\{d_j\}\| = 1$, i.e., $\|\Lambda\| \leqslant \|D_1^2\| \leqslant 24$. For the operator Γ we have, respectively, $N = d$, $n = 1$, $d_j = 1$ [see (1.5)], i.e., $\|\Gamma\| \leqslant 4d$. This completes the proof of the inequalities (3.15) and the lemma. ▮

We will also need the following general statement concerning the existence of a gap in the spectrum of an operator.

Lemma 5. Suppose that a self-ajoint operator A has a gap of length not less than L, i.e., there are λ_1 and λ_2 such that $\lambda_1, \lambda_2 \in \sigma(A)$, $(\lambda_1, \lambda_2) \cap \sigma(A) = \varnothing$, and $\lambda_2 \geqslant L + \lambda_1$. Then if B is a self-adjoint operator such that $\|B\| < L/2$, then $A + B$ has a gap (of positive length) in the spectrum.

Proof. Let $\lambda = (\lambda_1 + \lambda_2)/2$. Then according to the conditions of the lemma we have $\|(A - \lambda)^{-1}\| \leqslant 2/L$. From this and $\|B\| < L/2$ we easily obtain that the operator $(A + B - \lambda)^{-1}$ is a bounded operator, i.e., λ is not in the spectrum of $A + B$. On the hand, we can show that $\sigma(A + B) \cap (\lambda_2 - L/2, \lambda_2 + L/2) \neq \varnothing$. Indeed, assume that this is not true. Then representing A as $(A + B) - B$ and reasoning as before, we come up with the statement that $\lambda_2 \notin \sigma(A)$ which contradicts the assumptions of the lemma. That is, there is a μ_2 such that $\lambda < \mu_2$ and $\mu_2 \in \sigma(A + B)$. In same fashion we can find a μ_1 such that $\mu_1 < \lambda$ and $\mu_1 \in \sigma(A + B)$. Therefore $A + B$ has at least one gap and λ is inside of it. The lemma is proved. ∎

Proof of Theorem 2. The statement of the theorem follows from Lemma 5 (where $A = \mathfrak{A}^{(0)}$ and $B = \xi^{-1}\mathfrak{A}_{\mathscr{F}}$) and the estimates of Lemmas 2 and 4. ∎

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