ON THE LAPLACIAN IN THE HALFSPACE WITH A PERIODIC BOUNDARY CONDITION

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Abstract. We study spectral and scattering properties of the Laplacian $H^{(\sigma)} = -\Delta$ in $L_2(\mathbb{R}^{d+1}_+)$ corresponding to the boundary condition $\frac{\partial u}{\partial \nu} + \sigma u = 0$ with a periodic function σ. For non-negative σ we prove that $H^{(\sigma)}$ is unitarily equivalent to the Neumann Laplacian $H^{(0)}$. In general, there appear additional channels of scattering due to surface states. We prove absolute continuity of the spectrum of $H^{(\sigma)}$ under mild assumptions on σ.

Introduction

0.1. The present paper continues our study of the Laplacian on a halfspace with a periodic perturbation on the boundary. We consider the operator

$$H^{(\sigma)}u = -\Delta u \qquad \text{on } \mathbb{R}^{d+1}_+ := \{(x,y) \in \mathbb{R}^d \times \mathbb{R} : y > 0\} \tag{0.1}$$

together with a boundary condition of the third type

$$\frac{\partial u}{\partial \nu} + \sigma u = 0 \qquad \text{on } \mathbb{R}^d \times \{0\}. \tag{0.2}$$

Here ν denotes the exterior unit normal and $\sigma : \mathbb{R}^d \to \mathbb{R}$ is a $(2\pi\mathbb{Z})^d$-periodic function. Under the condition

$$\begin{array}{lll} \sigma \in L_{q,loc}(\mathbb{R}) & \text{for some } q > 1 & \text{if } d = 1, \\ \sigma \in L^0_{d,\infty,loc}(\mathbb{R}^d) & & \text{if } d \geq 2, \end{array} \tag{0.3}$$

(see Subsection 1.2 for weak L_p-spaces) $H^{(\sigma)}$ can be defined as a self-adjoint operator in $L_2(\mathbb{R}^{d+1}_+)$ by means of the quadratic form

$$\int_{\mathbb{R}^{d+1}_+} |\nabla u(x,y)|^2 \, dxdy + \int_{\mathbb{R}^d} \sigma(x) |u(x,0)|^2 \, dx, \qquad u \in H^1(\mathbb{R}^{d+1}_+).$$

Note that $H^{(\sigma)}$ can be viewed as a Schrödinger-type operator with the singular potential $\sigma(x)\delta(y)$ supported on $\mathbb{R}^d \times \{0\}$. In the physical interpretation this operator describes a quantum-mechanical particle interacting with the surface of a crystal.

Our goal is to study spectral and scattering properties of $H^{(\sigma)}$, viewing it as

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a (rather singular) perturbation of $H^{(0)}$, the Neumann Laplacian on $\mathbb{R}^{d+1}_+$. Let us describe our results. First we prove that the wave operators

$$W^{(\sigma)}_{\pm} := W_{\pm}(H^{(\sigma)}, H^{(0)}) = s - \lim_{t\to\pm\infty} \exp(itH^{(\sigma)}) \exp(-itH^{(0)})$$

exist and satisfy $\mathcal{R}(W^{(\sigma)}_{+}) = \mathcal{R}(W^{(\sigma)}_{-})$. However, in general the wave operators may *not* be complete due to the existence of surface states, i.e., states that are localized near the boundary for all time. We give sufficient conditions both for the completeness and for the non-completeness of the wave operators. If

$$\sigma(x) \geq 0, \qquad \text{a.e. } x \in \mathbb{R}^d, \tag{0.4}$$

we prove that there exist no surface states. Then the wave operators are unitary and provide a unitary equivalence between $H^{(\sigma)}$ and $H^{(0)}$.
On the other hand, if

$$\int_{(-\pi,\pi)^d} \sigma(x)\, dx \leq 0, \qquad \sigma \not\equiv 0,$$

we prove that there exist surface states and that they produce additional bands in the negative spectrum of $H^{(\sigma)}$. It is natural to ask whether the spectrum of $H^{(\sigma)}$ is still absolutely continuous in the presence of surface states. We prove that this is indeed the case under the assumption (0.3) if $d \leq 4$ and under the mild additional assumption

$$\sigma \in L^0_{2(d-2),\infty,loc}(\mathbb{R}^d) \qquad \text{if } d \geq 5.$$

Hence surface states correspond to *additional channels of scattering.*

0.2. Let us explain some of the mathematical ideas involved. By means of Floquet theory we represent $H^{(\sigma)}$ as a direct integral

$$\int_{[-\frac{1}{2},\frac{1}{2}]^d} \oplus H^{(\sigma)}(k)\, dk$$

with operators $H^{(\sigma)}(k)$ acting in $L_2(\Pi)$ where $\Pi := (-\pi,\pi)^d \times \mathbb{R}_+$ is a halfcylinder. The investigation of the operator $H^{(\sigma)}$ reduces to the study of the fibers $H^{(\sigma)}(k)$. Note that the fundamental domain Π is unbounded, so the operators $H^{(\sigma)}(k)$ have continuous spectrum. This part can be studied by scattering theory. To prove the absolute continuity of the spectrum of $H^{(\sigma)}$ we cannot (directly) apply the Thomas approach, since eigenvalues of $H^{(\sigma)}(k)$ may be embedded in the continuous spectrum. We "separate" them from the remaining spectrum by characterizing them, in the spirit of the Birman-Schwinger principle, as parameters λ for which a pseudo-differential operator $B^{(\sigma)}(\lambda, k)$ on the boundary $(-\pi,\pi)^d \times \{0\}$ has eigenvalue 0. The latter operator has discrete spectrum and can be handled by Thomas' method.

0.3. The case $d = 1$ has been treated in [Fr], [FrSh]. However, we have tried to make the presentation self-contained and we refer to those papers only for a few technical details.
When $d \geq 2$ additional difficulties arise. In particular, for the proof of absolute continuity we have to use the refined estimates of Lemma 3.4 and, if $d \geq 5$, we have to impose an additional condition on σ. Moreover, we have succeeded here to fit our problem into the framework of "smooth" scattering theory. This gives a rather short proof of both the existence and completeness of the wave operators and of the absence of singular continuous spectrum on the halfcylinder, and has probably applications to other problems with perturbations on surfaces.

0.4. The characteristic feature of partially periodic systems is the appearance of surface states, see [FrSh] and references therein. A substantial open problem is to prove that these states are not bound but correspond to additional channels of scattering, i.e., that the spectrum of the corresponding operator is purely absolutely continuous. Apart from the present paper we are only aware of [FiKl1], [FiKl2], [FrSh] dealing with this problem.

0.5. Let us briefly describe the structure of this paper. We state our main result about the operators $H^{(\sigma)}$ in Subsection 1.3 and reduce them in Subsection 1.5 to statements about the fiber operators $H^{(\sigma)}(k)$. Section 2 deals with their continuous spectrum, Section 3 with their point spectrum. Finally, in Section 4 we discuss the phenomenon of additional channels of scattering in more detail.

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1. Setting of the problem. The main results

1.1. **Notation.** In the halfspace $\mathbb{R}^{d+1}_+ = \{(x,y) \in \mathbb{R}^d \times \mathbb{R} : \ y > 0\}$ we consider the lattice $(2\pi\mathbb{Z})^d \times \{0\}$. A fundamental domain is the *halfcylinder*

$$\Pi := \{(x,y) \in \mathbb{R}^{d+1}_+ \,:\, x \in (-\pi,\pi)^d\}.$$

We think of the torus $\mathbb{T}^d := (\mathbb{R}/2\pi\mathbb{Z})^d$ as $[-\pi,\pi]^d$ with opposite edges identified, and write $Q^d := [-\frac{1}{2},\frac{1}{2}]^d$.
We use the notation $D = (D_x, D_y) = (-i\nabla_x, -i\frac{\partial}{\partial y})$ in $\mathbb{R}^{d+1}$.
For an open set $\Omega \subset \mathbb{R}^n$ the index in the notation of the norm $\|.\|_{L_2(\Omega)}$ is usually dropped. The space $L_2(\mathbb{T}^d)$ may be formally identified with

$L_2((-\pi,\pi)^d)$. We define the Fourier transformation $\mathcal{F}: L_2(\mathbb{T}^d) \to l_2(\mathbb{Z}^d)$ by

$$(\mathcal{F}f)_n = \hat{f}_n := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{T}^d} f(x) e^{-i\langle n,x\rangle}\, dx, \qquad n \in \mathbb{Z}^d.$$

Next, $H^s(\Omega)$ is the Sobolev space of order $s \in \mathbb{R}$ (with integrability index 2). By $H^s(\mathbb{T}^d)$ we denote the closure of $C^\infty(\mathbb{T}^d)$ in $H^s((-\pi,\pi)^d)$. Here $C^\infty(\mathbb{T}^d)$ is the space of functions in $C^\infty((-\pi,\pi)^d)$ which can be extended periodically to functions in $C^\infty(\mathbb{R}^d)$. The space $H^s(\mathbb{T}^d)$ is endowed with the norm

$$\|f\|^2_{H^s(\mathbb{T}^d)} := \sum_{n\in\mathbb{Z}^d} (1+|n|^2)^s |\hat{f}_n|^2, \qquad f \in H^s(\mathbb{T}^d).$$

By $\tilde{H}^s(\Pi)$ we denote the closure of $\tilde{C}^\infty(\Pi) \cap H^s(\Pi)$ in $H^s(\Pi)$. Here $\tilde{C}^\infty(\Pi)$ is the space of functions in $C^\infty(\Pi)$ which can be extended periodically with respect to x to functions in $C^\infty(\mathbb{R}^{d+1}_+)$.
We denote by $\mathcal{D}[a]$ the domain of a quadratic form a and by $\mathcal{D}(A)$, $\mathcal{N}(A)$, $\mathcal{R}(A)$ the domain, kernel and range, respectively, of a linear operator A.
Statements and formulae which contain the double index "$\pm$" are understood as two independent assertions.

1.2. **Weak L_p-spaces. Multiplication on the boundary.** We recall the definition of weak L_p-spaces on a measure space (X,μ). For a measurable function f on X put $\rho_f(t) := \mu(\{x \in X : |f(x)| > t\})$, $t > 0$, and

$$|f|_{p,\infty} := \sup_{t>0} t(\rho_f(t))^{1/p}, \qquad 1 \le p < \infty.$$

Then the weak L_p-spaces are defined by

$$L_{p,\infty}(X,\mu) := \{f : X \to \mathbb{C} : f \text{ measurable}, |f|_{p,\infty} < \infty\}.$$

We need also their subspaces

$$L^0_{p,\infty}(X,\mu) := \{f \in L_{p,\infty}(X,\mu) : \lim_{t\to 0} t(\rho_f(t))^{1/p} = \lim_{t\to\infty} t(\rho_f(t))^{1/p} = 0\}.$$

(Note that $\rho_f(t) = o(t^p)$ as $t \to 0$ if $\mu(X) < \infty$.)
We are interested in the following cases. When $X = \mathbb{T}^d$ and μ is the induced Lebesgue measure we write only $L_{p,\infty}(\mathbb{T}^d)$, $L^0_{p,\infty}(\mathbb{T}^d)$, and when $X = \mathbb{Z}^d$ and μ is the counting measure we write $l_{p,\infty}(\mathbb{Z}^d)$, $l^0_{p,\infty}(\mathbb{Z}^d)$.
The following quantitative embedding result was established in [BKaS].

Proposition 1.1. *Let $p > 2$ and $f \in L_{p,\infty}(\mathbb{T}^d)$, $a \in l_{p,\infty}(\mathbb{Z}^d)$. Then the operator $f\mathcal{F}^*a : l_2(\mathbb{Z}) \to L_2(\mathbb{T}^d)$ is bounded with*

$$\|f\mathcal{F}^*a\| \le c_{p,d} |f|_{p,\infty} |a|_{p,\infty}.$$

Moreover, if either $f \in L^0_{p,\infty}(\mathbb{T}^d)$ or $a \in l^0_{p,\infty}(\mathbb{Z}^d)$, then $f\mathcal{F}^*a$ is compact.

Now let σ be a periodic function satisfying

$$\begin{aligned} &\sigma \in L_q(\mathbb{T}) \quad \text{for some } q > 1 && \text{if } d = 1, \\ &\sigma \in L^0_{d,\infty}(\mathbb{T}^d) && \text{if } d \ge 2. \end{aligned} \tag{1.1}$$

Applying Proposition 1.1 with $f := \sqrt{|\sigma|}$ and $a_n := (1+|n|^2)^{-1/4}$, $n \in \mathbb{Z}^d$, we find that the form $\int_{\mathbb{T}^d} |\sigma(x)||f(x)|^2\,dx$, $f \in H^{1/2}(\mathbb{T}^d)$, is compact in $H^{1/2}(\mathbb{T}^d)$ and, consequently, that for every $\epsilon > 0$ there exists $C_1(\epsilon, d, \sigma) > 0$ such that

$$\int_{\mathbb{T}^d} |\sigma(x)||f(x)|^2\,dx \le \epsilon \|f\|^2_{H^{1/2}(\mathbb{T}^d)} + C_1(\epsilon, d, \sigma)\|f\|^2, \quad f \in H^{1/2}(\mathbb{T}^d). \tag{1.2}$$

From this we obtain

Corollary 1.2. *Assume σ satisfies* (1.1) *and let $\epsilon > 0$. Then there exists $C_2(\epsilon, d, \sigma) > 0$ such that*

$$\int_{(-\pi,\pi)^d} |\sigma(x)||u(x,0)|^2 dx \le \epsilon \|u\|^2_{H^1(\Pi)} + C_2(\epsilon, d, \sigma)\|u\|^2, \ \ u \in H^1(\Pi), \tag{1.3}$$

$$\int_{\mathbb{R}^d} |\sigma(x)||u(x,0)|^2 dx \le \epsilon \|u\|^2_{H^1(\mathbb{R}^{d+1}_+)} + C_2(\epsilon, d, \sigma)\|u\|^2, \ u \in H^1(\mathbb{R}^{d+1}_+). \tag{1.4}$$

Proof. First we note that an inequality like (1.2) holds with a possibly larger constant $\tilde{C}_1(\epsilon, d, \sigma)$ for all $f \in H^{1/2}((-\pi,\pi)^d)$. (This can be seen by using an extension operator $H^{1/2}((-\pi,\pi)^d) \to H^{1/2}(\alpha\mathbb{T}^d)$, $\alpha > 1$, and applying (1.2) with $\mathbb{T}^d$ replaced by $\alpha\mathbb{T}^d$.) Then (1.3) follows because of the boundedness of the trace operator $H^1(\Pi) \to H^{1/2}((-\pi,\pi)^d)$, and (1.4) follows from (1.3) by summation over all translates $\Pi + n$, $n \in \mathbb{Z}^d$. ☐

1.3. **The operators $H^{(\sigma)}$ on the halfplane. Main results.** Let σ be a real-valued periodic function satisfying (1.1). According to (1.4) the quadratic form

$$\begin{aligned} &\mathcal{D}[h^{(\sigma)}] := H^1(\mathbb{R}^{d+1}_+), \\ &h^{(\sigma)}[u] := \int_{\mathbb{R}^{d+1}_+} |Du(x,y)|^2\,dxdy + \int_{\mathbb{R}^d} \sigma(x)|u(x,0)|^2\,dx. \end{aligned} \tag{1.5}$$

is lower semibounded and closed in the Hilbert space $L_2(\mathbb{R}^{d+1}_+)$, so it generates a self-adjoint operator $H^{(\sigma)}$. The case $\sigma = 0$ corresponds to the *Neumann Laplacian* on the halfplane, whereas the case $\sigma \ne 0$ implements a (generalized) *boundary condition of the third type.*

The spectrum of the "unperturbed" operator $H^{(0)}$ coincides with $[0, +\infty)$ and is purely absolutely continuous of infinite multiplicity.

We begin our study of $H^{(\sigma)}$ with the investigation of the *wave operators*

$$W^{(\sigma)}_\pm := W_\pm(H^{(\sigma)}, H^{(0)}) = s - \lim_{t\to\pm\infty} \exp(itH^{(\sigma)})\exp(-itH^{(0)}). \tag{1.6}$$

(For the abstract mathematical scattering theory see, e.g., [Ya].)

Theorem 1.3. *Assume that σ satisfies* (1.1). *Then the wave operators $W^{(\sigma)}_\pm$ exist and satisfy $\mathcal{R}(W^{(\sigma)}_+) = \mathcal{R}(W^{(\sigma)}_-)$.*

However, in general the wave operators will not be complete. There may appear additional bands in the spectrum of $H^{(\sigma)}$, which correspond to *surface states*. See Section 4 for a detailed discussion of this phenomenon. Under the mild additional (if $d \geq 5$) assumption

$$\begin{aligned} &\sigma \in L_q(\mathbb{T}) \quad \text{for some } q > 1 && \text{if } d = 1, \\ &\sigma \in L^0_{d,\infty}(\mathbb{T}^d) && \text{if } 2 \leq d \leq 4, \\ &\sigma \in L^0_{2(d-2),\infty}(\mathbb{T}^d) && \text{if } d \geq 5, \end{aligned} \tag{1.7}$$

we are able to prove that the spectrum of the operator $H^{(\sigma)}$ is absolutely continuous.

Theorem 1.4. *Assume that σ satisfies* (1.7)*. Then the operator $H^{(\sigma)}$ has purely absolutely continuous spectrum.*

Therefore surface states correspond to *additional channels of scattering.* In Section 4 we give a sufficient condition for the existence of surface states. Conversely, if

$$\sigma(x) \geq 0 \qquad \text{a.e. } x \in \mathbb{R}^d, \tag{1.8}$$

there exist no surface states and we obtain a rather complete result.

Theorem 1.5. *Assume that σ satisfies* (1.1) *and* (1.8)*. Then the wave operators $W_\pm^{(\sigma)}$ are unitary and satisfy*

$$H^{(\sigma)} = W_\pm^{(\sigma)} H^{(0)} W_\pm^{(\sigma)*}. \tag{1.9}$$

We would like to mention the following simple extension.

Remark 1.6. Our results remain valid if σ is periodic with respect to an arbitrary d-dimensional lattice in $\mathbb{R}^d$. After a change of variables this amounts to replace the differential operator $-\Delta$ above by $D_x^* a D_x + D_y^2$ with a positive definite $(d \times d)$-matrix a. All our arguments extend to this case.

Remark 1.7. One might conjecture that Theorem 1.4 remains valid under the assumption (1.1).

1.4. **The operators $H^{(\sigma)}(k)$ on the halfcylinder. Direct Integral Decomposition.** Let σ be a real-valued periodic function satisfying (1.1) and let $k \in Q^d$. According to (1.3) the quadratic form

$$\begin{aligned} &\mathcal{D}[h^{(\sigma)}(k)] := \tilde{H}^1(\Pi), \\ &h^{(\sigma)}(k)[u] := \int_\Pi \left(|(D_x + k)u(x,y)|^2 + |D_y u(x,y)|^2 \right) dxdy + \\ &\qquad\qquad + \int_{\mathbb{T}^d} \sigma(x) |u(x,0)|^2 \, dx. \end{aligned} \tag{1.10}$$

is lower semibounded and closed in the Hilbert space $L_2(\Pi)$, so it generates a self-adjoint operator $H^{(\sigma)}(k)$. In addition to the Neumann (if $\sigma = 0$) or third type (if $\sigma \neq 0$) boundary condition at $(-\pi, \pi)^d \times \{0\}$, the functions in

$\mathcal{D}(H^{(\sigma)}(k))$ satisfy periodic boundary conditions at $\partial(-\pi,\pi)^d \times \mathbb{R}_+$.
The operator $H^{(\sigma)}$ on the halfplane can be partially diagonalized by means of the *Gelfand transformation.* This operator is initially defined for $u \in \mathcal{S}(\mathbb{R}_+^{d+1})$, the Schwartz class on $\mathbb{R}_+^{d+1}$, by

$$(\mathcal{U}u)(k,x,y) := \sum_{n\in\mathbb{Z}^d} e^{-i\langle k,x+2\pi n\rangle} u(x+2\pi n,y), \qquad k\in Q^d,\ (x,y)\in\Pi,$$

and extended by continuity to a *unitary* operator

$$\mathcal{U} : L_2(\mathbb{R}_+^{d+1}) \to \int_{Q^d} \oplus L_2(\Pi)\, dk. \tag{1.11}$$

As in the case $d=1$ (cf. [Fr]) one finds that

$$\mathcal{U}\, H^{(\sigma)}\, \mathcal{U}^* = \int_{Q^d} \oplus H^{(\sigma)}(k)\, dk. \tag{1.12}$$

This relation allows us to investigate the operator $H^{(\sigma)}$ by studying the fibers $H^{(\sigma)}(k)$.
We will now state our main results about the operators $H^{(\sigma)}(k)$. In the next subsection we will show how the proofs of the theorems from Section 1.3 can be reduced to these results.
In Section 2 we study the continuous spectrum of $H^{(\sigma)}(k)$ and the wave operators

$$W_\pm^{(\sigma)}(k) := W_\pm(H^{(\sigma)}(k), H^{(0)}(k)) = s\!-\!\lim_{t\to\pm\infty} \exp(itH^{(\sigma)}(k)) \exp(-itH^{(0)}(k)).$$

We will prove

Theorem 1.8. *Assume that σ satisfies* (1.1) *and let $k\in Q^d$. Then the wave operators $W_\pm^{(\sigma)}(k)$ exist and are complete. In particular, $\sigma_{ac}\big(H^{(\sigma)}(k)\big) = [|k|^2,+\infty)$.*
Moreover, $\sigma_{sc}\left(H^{(\sigma)}(k)\right) = \emptyset$.

In Section 3 we investigate the point spectrum of the operators $H^{(\sigma)}(k)$ and prove

Theorem 1.9. *Assume that σ satisfies* (1.1) *and let $k\in Q^d$. Then $\sigma_p\left(H^{(\sigma)}(k)\right)$ (if not empty) consists of eigenvalues of finite multiplicities which may accumulate at $+\infty$ only. If σ satifies in addition* (1.8)*, then $\sigma_p\left(H^{(\sigma)}(k)\right) = \emptyset$.*

Note that the case of an infinite sequence of (embedded) eigenvalues actually occurs (see Example 3.3).
To prove absolute continuity of the spectrum of $H^{(\sigma)}$ we have to control the k-dependence of the eigenvalues of $H^{(\sigma)}(k)$. In Subsection 3.4 we prove the technical

Proposition 1.10. *Assume that σ satisfies* (1.7)*. Then there exists a countable number of domains $U_j\subset\mathbb{R}$, $V_j\subset\mathbb{R}^d$ and real-analytic functions $h_j : U_j\times V_j \to \mathbb{R}$ satisfying*

(1) *for all* $k \in Q^d$ *and* $\lambda \in \sigma_p\left(H^{(\sigma)}(k)\right)$ *there is a* j *such that* $(\lambda, k) \in U_j \times V_j$ *and* $h_j(\lambda, k) = 0$, *and*
(2) *for all* j *and all* $\lambda \in U_j$ *one has* $h_j(\lambda, .) \not\equiv 0$.

1.5. **Reduction to the halfcylinder.** Assuming Theorems 1.8, 1.9 and Proposition 1.10 we give now the proofs of Theorems 1.3, 1.4, 1.5.

Proof of Theorem 1.3. Using Theorem 1.8 one easily finds that the limit (1.6) exists and satisfies

$$W_\pm^{(\sigma)} = \mathcal{U}^* \left(\int_{Q^d} \oplus W_\pm^{(\sigma)}(k)\, dk \right) \mathcal{U}. \tag{1.13}$$

Moreover, because of the completeness of $W_\pm^{(\sigma)}(k)$,

$$\mathcal{R}(W_\pm^{(\sigma)}) = \mathcal{U}^* \left(\int_{Q^d} \oplus \mathcal{R}(P_{ac}^{(\sigma)}(k))\, dk \right) \mathcal{U},$$

where $P_{ac}^{(\sigma)}(k)$ denotes the projection onto the absolutely continuous subspace of $H^{(\sigma)}(k)$. This completes the proof of Theorem 1.3. □

Proof of Theorem 1.4. We follow the approach suggested in [FiKl1]. Let $\Lambda \subset \mathbb{R}$ with $\operatorname{meas}\Lambda = 0$. Denoting the spectral projections of $H^{(\sigma)}$, $H^{(\sigma)}(k)$ corresponding to Λ by $E^{(\sigma)}(\Lambda)$, $E^{(\sigma)}(\Lambda, k)$, it follows from (1.12) that

$$\mathcal{U}\, E^{(\sigma)}(\Lambda)\, \mathcal{U}^* = \int_{Q^d} \oplus E^{(\sigma)}(\Lambda, k)\, dk$$

and we have to prove that this operator is equal to 0.
For this we write $Q^d = K_1 \cup K_2$ where

$$K_1 := \left\{ k \in Q^d :\ \sigma_p\left(H^{(\sigma)}(k)\right) \cap \Lambda = \emptyset \right\}, \qquad K_2 := Q^d \setminus K_1.$$

Since $\sigma_{sc}\left(H^{(\sigma)}(k)\right) = \emptyset$ by Theorem 1.8, we immediately obtain $E^{(\sigma)}(\Lambda, k) = 0$ for $k \in K_1$. Now we note that with the notation of Proposition 1.10

$$K_2 \subset \bigcup_j \{ k \in V_j \cap Q^d :\ h_j(\lambda, k) = 0 \quad \text{for some } \lambda \in U_j \cap \Lambda \}.$$

It follows from property (2) there and an abstract result about analytic functions (cf., e.g., [FiKl1]) that $\operatorname{meas} K_2 = 0$. This completes the proof of Theorem 1.4. □

Proof of Theorem 1.5. It follows from Theorems 1.8, 1.9 that under the assumption (1.8) the operators $H^{(\sigma)}(k)$ have purely absolutely continuous spectrum. So the wave operators $W_\pm^{(\sigma)}(k)$ are not only complete but unitary, and $W_\pm^{(\sigma)}$ is unitary by (1.13). Relation (1.9) is the intertwining property of the wave operators. This completes the proof of Theorem 1.5. □

2. The continuous spectrum of the operators $H^{(\sigma)}(k)$

2.1. **Scattering for relatively smooth perturbations.** Our proof of Theorem 1.8 is based on the "smooth" scattering theory by Kato-Kuroda. For the reader's convenience we will recall here some notions and results we will use. Our exposition follows [Ya]. All Hilbert spaces that appear are assumed to be separable.

Let H_0 be a self-adjoint operator in a Hilbert space $\mathfrak{H}$. Denote by $E_0(X)$ the spectral projection of H_0 corresponding to a measurable set $X \subset \mathbb{R}$. We fix a compact interval Λ such that the spectrum of H_0 on Λ is purely absolutely continuous of constant multiplicity $N \in \mathbb{N} \cup \{\infty\}$ and a unitary operator $\Phi : \mathcal{R}(E_0(\Lambda)) \to L_2(\Lambda, \mathbb{C}^N)$ which diagonalizes H_0 on Λ, i.e., $\Phi E_0(X)\Phi^*$ is the operator of multiplication by the characteristic function χ_X for any measurable set $X \subset \Lambda$. (Here $\mathbb{C}^N = l_2(\mathbb{N})$ if $N = \infty$.)

Let $\mathfrak{G}$ be an "auxiliary" Hilbert space and let $G_0 : \mathfrak{H} \to \mathfrak{G}$ be a $|H_0|^{1/2}$-compact operator, i.e., $\mathcal{D}(G_0) \supset \mathcal{D}(|H_0|^{1/2})$ and $G_0(|H_0|^{1/2} + I)^{-1}$ is compact. Then $\Phi(G_0E_0(\Lambda))^*$ is a (compact) operator from $\mathfrak{G}$ into $L_2(\Lambda, \mathbb{C}^N)$. We recall that G_0 is called *strongly H_0-smooth* on Λ (with exponent 1) if $\Phi(G_0E_0(\Lambda))^*$ maps $\mathfrak{G}$ continuously into $C^{0,1}(\Lambda, \mathbb{C}^N)$, i.e., if there exists a $C > 0$ such that for all $g \in \mathfrak{G}$ and $f := (G_0E_0(\Lambda))^*g$

$$\sup_{\lambda\in\Lambda} |\Phi f(\lambda)| + \sup_{\lambda\neq\nu\in\Lambda} \frac{|\Phi f(\lambda) - \Phi f(\nu)|}{|\lambda - \nu|} \le C\|g\|.$$

Now let H be another self-adjoint operator in $\mathfrak{H}$ with

$$\mathcal{D}(|H|^{1/2}) = \mathcal{D}(|H_0|^{1/2}).$$

Moreover, assume that there exists a $|H_0|^{1/2}$-compact operator $G : \mathfrak{H} \to \mathfrak{G}$ such that

$$(Hf, f_0) = (f, H_0f_0) + (Gf, G_0f_0) = (f, H_0f_0) + (G_0f, Gf_0)$$

for all $f \in \mathcal{D}(H)$, $f_0 \in \mathcal{D}(H_0)$. Then the main result of the "smooth" scattering theory can be summarized as follows.

Proposition 2.1. *Assume that there are compact intervals Λ_n, $n \in \mathbb{N}$, such that $\sigma(H_0)\setminus\bigcup_{n\in\mathbb{N}} \Lambda_n$ is discrete and such that G_0, G are strongly H_0-smooth on each Λ_n. Then the wave operators $W_\pm(H, H_0)$ exist and are complete. Moreover, if $\mathcal{N}(G) = \{0\}$, then $\sigma_{sc}(H) = \emptyset$.*

The proof can be found in [Ya] (see in particular Theorems 4.6.5 and 4.7.9). Note that under the assumptions of the proposition we have also rather detailed information about the eigenvalues of H (see Theorem 4.7.10 in [Ya]).

In our application the operator G will not be injective, but we can use the following

Lemma 2.2. *In the situation of Proposition 2.1, but without any assumption on $\mathcal{N}(G)$, suppose there exists a Hilbert space $\mathfrak{A}$ and a $|H_0|^{1/2}$-compact* *operator $A : \mathfrak{H} \to \mathfrak{A}$ with $\mathcal{N}(A) = \{0\}$ which is strongly H_0-smooth on each Λ_n. Then $\sigma_{sc}(H) = \emptyset$.*

Proof. It suffices to apply Proposition 2.1 with the auxiliary space $\tilde{\mathfrak{G}} := \mathfrak{G} \oplus \mathfrak{A}$ and the operators $\tilde{G_0}, \tilde{G} : \mathfrak{H} \to \tilde{\mathfrak{G}}$,

$$\tilde{G_0} f := (G_0 f, 0), \qquad \tilde{G} f := (Gf, Af),$$

with domains $\mathcal{D}(\tilde{G_0}) := \mathcal{D}(G_0)$, $\mathcal{D}(\tilde{G}) := \mathcal{D}(G) \cap \mathcal{D}(A)$. □

2.2. **Diagonalization of the unperturbed operators $H^{(0)}(k)$.** We fix $k \in Q^d$. In order to apply the method of Subsection 2.1 we need a rather explicit spectral representation of the unperturbed operator $H^{(0)}(k)$. Applying a Fourier transformation with respect to the variable x and a Fourier cosine transformation with respect to the variable y we find that the spectrum of $H^{(0)}(k)$ is purely absolutely continuous and coincides with $[|k|^2, +\infty)$. The spectral multiplicity of a point λ is

$$N(\lambda, k) := \sharp\{n \in \mathbb{Z}^d : |n + k|^2 \leq \lambda\}.$$

In particular, the spectral multiplicity is piecewise constant and changes at the points of the *threshold set*

$$\tau(k) := \{|n + k|^2 : n \in \mathbb{Z}^d\}.$$

We realize now $H^{(0)}(k)$ as multiplication by the independent variable λ in

$$\mathfrak{h}(k) := \int_{|k|^2}^{+\infty} \oplus\, \mathbb{C}^{N(\lambda,k)}\, d\lambda.$$

We write elements in $\mathbb{C}^{N(\lambda,k)}$ as sequences $a \in l_2(\mathbb{Z}^d)$ such that $a_n = 0$ for $|n + k|^2 > \lambda$. The operator $\Gamma(k) : L_2(\Pi) \to \mathfrak{h}(k)$, defined originally on functions $u \in \tilde{C}^\infty(\Pi)$ with bounded support by

(2.1)
$$(\Gamma(k)u)_n(\lambda) := \\ = \frac{1}{(2\pi)^{d/2}\sqrt{\pi}\sqrt[4]{\lambda - |n+k|^2}} \int_\Pi u(x,y) e^{-i\langle n,x\rangle} \cos(\sqrt{\lambda - |n+k|^2}\, y)\, dx dy, \\ |n + k|^2 < \lambda,$$

extends by continuity to a *unitary* operator. (That $(\Gamma(k)u)(\lambda)$ is not completely defined for $\lambda \in \tau(k)$ is not important since $\mathrm{meas}(\tau(k)) = 0$.) Then $\Gamma(k)H^{(0)}(k)\Gamma(k)^*$ is the operator of multiplication with the independent variable λ in $\mathfrak{h}(k)$. In particular, the spectral projection $E^{(0)}(\Lambda, k)$ of $H^{(0)}(k)$

corresponding to a measurable set Λ is given by

(2.2)

$$(E^{(0)}(\Lambda,k)u)(x,y) := \\ = \frac{1}{(2\pi)^{d/2}} \sum_{n\in\mathbb{Z}^d} \left(\frac{1}{\sqrt{\pi}} \int_{\Lambda\cap(|n+k|^2,\infty)} \frac{(\Gamma(k)u)_n(\lambda)\cos(\sqrt{\lambda-|n+k|^2}\,y)}{\sqrt[4]{\lambda-|n+k|^2}}\,d\lambda \right) e^{i\langle n,x\rangle}, \\ (x,y)\in\Pi.$$

(As usual, convergence of the integral and of the sum are understood in the L_2-sense.)

2.3. **Proof of Theorem 1.8.** Again we fix $k \in Q^d$. We want to apply the method of Subsection 2.1 with $\mathfrak{G} := L_2(\mathbb{T}^d)$ and the operators $G_0, G : L_2(\Pi) \to L_2(\mathbb{T}^d)$ defined by

$$G_0 u := (\operatorname{sgn}\sigma)\sqrt{|\sigma|}\,u(.,0), \qquad Gu := \sqrt{|\sigma|}\,u(.,0),$$

on $\mathcal{D}(G_0) = \mathcal{D}(G) := \tilde{H}^1(\Pi)$. The operators G_0, G are compact from $\tilde{H}^1(\Pi)$ to $L_2(\mathbb{T}^d)$ by Proposition 1.1 and the continuity of the trace operator $\tilde{H}^1(\Pi) \to H^{1/2}(\mathbb{T}^d)$, and we have obviously

$$(H^{(\sigma)}(k)u,u_0) = (u,H^{(0)}(k)u_0) + (Gu,G_0u_0) = (u,H^{(0)}(k)u_0) + (G_0u,Gu_0)$$

for all $u,u_0 \in \tilde{H}^1(\Pi)$. Let us check strong $H^{(0)}(k)$-smoothness.

Lemma 2.3. *The operators G_0, G are strongly $H^{(0)}(k)$-smooth on any compact interval $\Lambda \subset \mathbb{R}\setminus\tau(k)$.*

Proof. We consider G only. For any $\Lambda \subset \mathbb{R}\setminus\tau(k)$ we find easily from (2.1), (2.2) that

$$(\Gamma(k)(GE^{(0)}(\Lambda,k))^*f)_n(\lambda) = \\ = \frac{1}{(2\pi)^{d/2}\sqrt{\pi}\sqrt[4]{\lambda-|n+k|^2}} \int_{\mathbb{T}^d} \sqrt{|\sigma(x)|}\,f(x)e^{-i\langle n,x\rangle}\,dx,$$

for $f \in L_2(\mathbb{T}^d)$ and $\lambda \in \Lambda$, $|n+k|^2 < \lambda$. Noting that

$$\left| \int_{\mathbb{T}^d} \sqrt{|\sigma(x)|}\,f(x)e^{-i\langle n,x\rangle}\,dx \right| \le \|\sigma\|_{L_1}^{1/2}\|f\|,$$

we obtain the assertion. ☐

To apply Lemma 2.2 we need a strongly $H^{(0)}(k)$-smooth operator which is injective. Put $\mathfrak{A} := L_2(\Pi)$ and $A : L_2(\Pi) \to L_2(\Pi)$,

$$(Au)(x,y) := \eta(y)u(x,y), \qquad (x,y)\in\Pi,$$

where η is a measurable function on $\mathbb{R}_+$ satisfying

$$0 < \eta(y) \le C(1+|y|)^{-s}, \qquad y\in\mathbb{R}_+, \tag{2.3}$$

for some $s > \frac{3}{2}$, $C > 0$. Then A is injective and compact as operator from $\tilde{H}^1(\Pi)$ to $L_2(\Pi)$. Moreover, we have

Lemma 2.4. *The operator A is strongly $H^{(0)}(k)$-smooth on any compact interval $\Lambda \subset \mathbb{R} \setminus \tau(k)$.*

Proof. As in the previous proof we use (2.1), (2.2) to find

$$(\Gamma(k)(AE^{(0)}(\Lambda,k))^*u)_n(\lambda) = \frac{1}{(2\pi)^{d/2}\sqrt{\pi}\sqrt[4]{\lambda - |n+k|^2}} w_n(\sqrt{\lambda - |n+k|^2}),$$

where

$$w_n(\xi) := \int_\Pi \eta(y)u(x,y)e^{-i\langle n,x\rangle}\cos(\xi y)\,dxdy, \qquad \xi \in \mathbb{R}_+.$$

From (2.3) we get that $w_n \in H^s(\mathbb{R}_+)$ with $\|w_n\|_{H^s} \leq \tilde{C}\|u\|$. The assertion follows now from the embedding theorem since $s > \frac{3}{2}$. □

Finally, we can give the

Proof of Theorem 1.8. We write $[|k|^2, +\infty) \setminus \tau(k)$ as a countable union of compact intervals and apply Proposition 2.1 with G_0, G as above. This yields the existence and completeness of the wave operators $W_\pm^{(\sigma)}(k)$. To prove the absence of singular continuous spectrum we use Lemma 2.2 with A as above. □

3. The point spectrum of the operators $H^{(\sigma)}(k)$

3.1. **The operators $B^{(\sigma)}(\lambda,k)$ on the boundary. Characterization of eigenvalues of $H^{(\sigma)}(k)$.** Let σ be a real-valued periodic function satisfying (1.1) and let $\lambda \in \mathbb{R}$, $k \in Q^d$. In the Hilbert space $L_2(\mathbb{T}^d)$ we consider the quadratic forms

$$\begin{aligned} &\mathcal{D}[b^{(\sigma)}(\lambda,k)] := H^{1/2}(\mathbb{T}^d), \\ &b^{(\sigma)}(\lambda,k)[f] := \sum_{n\in\mathbb{Z}^d} \beta_n(\lambda,k)\,|\hat{f}_n|^2 + \int_{\mathbb{T}^d} \sigma(x)|f(x)|^2\,dx, \end{aligned} \tag{3.1}$$

where

$$\beta_n(\lambda,k) := \begin{cases} \sqrt{\sum_{j=1}^d (n_j+k_j)^2 - \lambda} & \text{if } \sum_{j=1}^d (n_j+k_j)^2 > \lambda, \\ -\sqrt{\lambda - \sum_{j=1}^d (n_j+k_j)^2} & \text{if } \sum_{j=1}^d (n_j+k_j)^2 \leq \lambda. \end{cases} \tag{3.2}$$

According to (1.2) the forms $b^{(\sigma)}(\lambda,k)$ are lower semibounded and closed, so they generate self-adjoint operators $B^{(\sigma)}(\lambda,k)$.
The compactness of the embedding of $H^{1/2}(\mathbb{T}^d)$ in $L_2(\mathbb{T}^d)$ implies that the operators $B^{(\sigma)}(\lambda,k)$ have compact resolvent.
Now we characterize the eigenvalues of the operator $H^{(\sigma)}(k)$ as the values λ for which 0 is an eigenvalue of the operators $B^{(\sigma)}(\lambda,k)$. More precisely, we have

Proposition 3.1. *Let $k \in Q^d$ and $\lambda \in \mathbb{R}$.*

(1) *Let* $u \in \mathcal{N}(H^{(\sigma)}(k) - \lambda I)$ *and define*

$$f(x) := u(x, 0), \qquad x \in \mathbb{T}^d. \tag{3.3}$$

Then $f \in \mathcal{N}(B^{(\sigma)}(\lambda, k))$, $\hat{f}_n = 0$ *if* $|n + k|^2 \leq \lambda$ *and, moreover,*

$$u(x, y) = \frac{1}{(2\pi)^{d/2}} \sum_{|n+k|^2 > \lambda} \hat{f}_n \, e^{i\langle n, x\rangle} \, e^{-\beta_n(\lambda,k)\, y}, \qquad (x, y) \in \Pi. \tag{3.4}$$

(2) *Let* $f \in \mathcal{N}(B^{(\sigma)}(\lambda, k))$ *such that* $\hat{f}_n = 0$ *if* $|n + k|^2 \leq \lambda$ *and define* u *by* (3.4).
Then $u \in \mathcal{N}(H^{(\sigma)}(k) - \lambda I)$ *and, moreover,* (3.3) *holds.*

The proof of this proposition is straightforward and will be omitted. (See [FrSh] for the case $d = 1$.)

Remark 3.2. Obviously, the statement of Proposition 3.1 does not depend on the definition of $\beta_n(\lambda, k)$ for $|n + k|^2 \leq \lambda$.

3.2. **Proof of Theorem 1.9.** Using Proposition 3.1 we can give now the

Proof of Theorem 1.9. Let $\Lambda = (\lambda_-, \lambda_+)$ be an open interval. A Birman-Schwinger-type argument as in [FrSh] using Proposition 3.1 and the monotonicity of $B^{(\sigma)}(\lambda, k)$ with respect to λ yields

$$\begin{aligned} &\sharp_{cm}\{\lambda \in (\lambda_-, \lambda_+) : \ \lambda \text{ is eigenvalue of } H^{(\sigma)}(k)\} \leq \\ &\leq \ \sharp_{cm}\{\mu < 0 : \ \mu \text{ is eigenvalue of } B^{(\sigma)}(\lambda_+, k)\} - \\ &\quad -\sharp_{cm}\{\mu \leq 0 : \ \mu \text{ is eigenvalue of } B^{(\sigma)}(\lambda_-, k)\}. \end{aligned} \tag{3.5}$$

Here $\sharp_{cm}\{...\}$ means that the cardinality of $\{...\}$ is determined according to multiplicities. The RHS of (3.5) is finite since $B^{(\sigma)}(\lambda_\pm, k)$ are lower semibounded and have compact resolvent. This proves the first part of the theorem.
Now assume (1.8) and let $\lambda \in \mathbb{R}$. If $f \in \mathcal{N}(B^{(\sigma)}(\lambda, k))$ satisfies $\hat{f}_n = 0$ for $|n + k|^2 \leq \lambda$, then

$$0 = b^{(\sigma)}(\lambda, k)[f] \geq \sum_{|n+k|^2 > \lambda} \beta_n(\lambda, k) |\hat{f}_n|^2$$

and therefore $f = 0$. So by Proposition 3.1 (1), $\lambda \notin \sigma_p\left(H^{(\sigma)}(k)\right)$. □

We end this subsection with an example of an infinite sequence of (embedded) eigenvalues.

Example 3.3. Let $\sigma \equiv \sigma_0 < 0$ be a negative constant and $k \in Q^d$. Then

$$\sigma_p\left(H^{(\sigma)}(k)\right) = \{-\sigma_0^2 + |n + k|^2 : \ n \in \mathbb{Z}^d\}.$$

This follows easily by Proposition 3.1 or directly by separation of variables.

3.3. **Complexification.** Throughout this subsection we fix $k = (k_1, k') \in Q^d$, $\lambda \in \mathbb{R} \setminus \tau(k)$ and assume

$$k_1 \neq 0.$$

All the constants in this subsection may depend on k, λ. To simplify the notation we agree to write $B^{(\sigma)}(\mu)$, $\beta_n(\mu)$ instead of $B^{(\sigma)}(\lambda, \mu e_1 + k')$, $\beta_n(\lambda, \mu e_1 + k')$. (Here $e_1 = (1, 0, \cdots, 0) \in \mathbb{R}^d$.)
Note that we can choose $\delta > 0$ such that

$$(n_1 + \mu)^2 + |n' + k'|^2 - \lambda \neq 0, \qquad n = (n_1, n') \in \mathbb{Z}^d,$$

for all $\mu \in \mathbb{C}$ with $|\mathrm{Re}\,\mu - k_1| < \delta$. We will also assume $\delta < |k_1|$. Therefore, the functions β_n, $n \in \mathbb{Z}^d$, originally defined on $[-\frac{1}{2}, \frac{1}{2}]$ (since λ, k' are fixed), admit a unique analytic continuation to

$$W := \{\mu \in \mathbb{C} : |\mathrm{Re}\,\mu - k_1| < \delta\}.$$

Then we can define sectorial and closed forms $b^{(\sigma)}(\mu)$ for $\mu \in W$ by (3.1). The corresponding m-sectorial operators $B^{(\sigma)}(\mu)$ form an analytic family of type (B) with respect to $\mu \in W$ (see, e.g., Section VII.4 in [K]).
Our goal in this subsection is to study the operators $B^{(\sigma)}(\mu)$ with large $|\mathrm{Im}\,\mu|$. We begin with the unperturbed case $\sigma = 0$ and consider the symbol $\beta(\mu) = (\beta_n(\mu))_{n \in \mathbb{Z}^d}$. Noting that

$$|\beta_n(\mu)|^4 = |(n_1 + \mathrm{Re}\,\mu)^2 - (\mathrm{Im}\,\mu)^2 + |n' + k'|^2 - \lambda|^2 + 4|\mathrm{Im}\,\mu|^2 |n_1 + \mathrm{Re}\,\mu|^2$$

for $n = (n_1, n') \in \mathbb{Z}^d$ and recalling the properties of δ we find easily that there is a $C_1 > 0$ such that

$$|\beta_n(\mu)| \geq \frac{1}{C_1}(1 + |\mathrm{Im}\,\mu|)^{1/2}, \qquad n \in \mathbb{Z}^d, \mu \in W. \tag{3.6}$$

This is an estimate of $\beta(\mu)$ in $l_\infty(\mathbb{Z}^d)$. We also need the following refined estimate in the class $l_{s,\infty}(\mathbb{Z}^d)$ from [BSu].

Lemma 3.4. *Let $d \geq 2$ and let k, λ, W be as above. Put $s := \max\{d, 2(d-2)\}$. Then there exists a $C_2 > 0$ such that*

$$|\beta(\mu)^{-1}|_{s,\infty} \leq C_2, \qquad \mu \in W.$$

Proof. When $\lambda = 0$ and $\mathrm{Im}\,\mu = \frac{1}{2}$, our $|\beta(\mu)|^{-1}$ coincides with $|h_0(\mathrm{Im}\,\mu)|^{-1/2}$ in [BSu] (up to multiples of 2π) and our lemma is a special case of Theorem 3.1 there. The extension to our situation is straightforward. □

The main result of this subsection is

Proposition 3.5. *Assume that σ satisfies* (1.7) *and let k, λ, W be as above. Then there exist η_0, $C_3 > 0$ such that for all $\mu \in W$ with $|Im\,\mu| > \eta_0$ the operator $B^{(\sigma)}(\mu)$ is boundedly invertible with*

$$\left\| \left(B^{(\sigma)}(\mu) \right)^{-1} \right\| \leq \frac{C_3}{(1 + |\mathrm{Im}\,\mu|)^{1/2}}. \tag{3.7}$$

Remark 3.6. If $d = 1$, then the exponent $\frac{1}{2}$ in the RHS of (3.7) can be replaced by 1, see [FrSh].

Proof. In view of the preceding remark we can assume $d \geq 2$. We have to find η_0, $C_3 > 0$ such that for all $0 \neq f \in H^{1/2}(\mathbb{T}^d)$, $\mu \in W$ with $|\operatorname{Im}\mu| > \eta_0$ there exists $0 \neq g \in H^{1/2}(\mathbb{T}^d)$ such that

$$|b^{(\sigma)}(\mu)[f,g]| \geq \frac{1}{C_3}(1 + |\operatorname{Im}\mu|)^{1/2}\|f\|\|g\|.$$

For given $0 \neq f \in H^{1/2}(\mathbb{T}^d)$, $\mu \in W$ we define g by its Fourier coefficients

$$\hat{g}_n := \frac{\beta_n(\mu)}{|\beta_n(\mu)|}\,\hat{f}_n, \qquad n \in \mathbb{Z}^d.$$

Then we have $0 \neq g \in H^{1/2}(\mathbb{T}^d)$,

$$\|g\| = \|f\|, \tag{3.8}$$

and

$$|b^{(\sigma)}(\mu)[f,g]| \geq \sum_{n\in\mathbb{Z}^d} |\beta_n(\mu)||\hat{f}_n|^2 - \tfrac{1}{2}\|\sqrt{|\sigma|}f\|^2 - \tfrac{1}{2}\|\sqrt{|\sigma|}g\|^2. \tag{3.9}$$

Because of (1.7) we can, for given $\epsilon > 0$, write $\sqrt{|\sigma|} = \rho_{1,\epsilon} + \rho_{2,\epsilon}$ with $\rho_{1,\epsilon} \in L_\infty(\mathbb{T}^d)$ and $|\rho_{2,\epsilon}|_{2s,\infty} < \epsilon$, $s := \max\{d, 2(d-2)\}$. Then by (3.6), Lemma 3.4 and Proposition 1.1

$$\begin{aligned}\|\sqrt{|\sigma|}f\| &\leq \\ &\leq \left(C_1^{1/2}(1 + |\operatorname{Im}\mu|)^{-1/4}\|\rho_{1,\epsilon}\|_\infty + c_{2s,d}C_2^{1/2}|\rho_{2,\epsilon}|_{2s,\infty}\right)\||B^{(0)}(\mu)|^{1/2}f\|.\end{aligned}$$

Now choose $\epsilon > 0$ small and then η_0 large such that

$$\|\sqrt{|\sigma|}f\|^2 \leq \tfrac{1}{2}\sum_{n\in\mathbb{Z}^d}|\beta_n(\mu)||\hat{f}_n|^2$$

for all $\mu \in W$ with $|\operatorname{Im}\mu| > \eta_0$. Using a similar estimate for $\|\sqrt{|\sigma|}g\|^2$ and (3.9), (3.6), (3.8) we arrive at

$$|b^{(\sigma)}(\mu)[f,g]| \geq \tfrac{1}{2}\sum_{n\in\mathbb{Z}^d}|\beta_n(\mu)||\hat{f}_n|^2 \geq \tfrac{1}{2C_1}(1 + |\operatorname{Im}\mu|)^{1/2}\|f\|\|g\|,$$

whenever $|\operatorname{Im}\mu| > \eta_0$, as claimed. □

3.4. **Proof of Proposition 1.10.** The core of Proposition 1.10 is contained in the following

Proposition 3.7. *Assume that σ satisfies (1.7) and let $k^0 \in Q^d$, $\lambda_0 \in \sigma_p\left(H^{(\sigma)}(k^0)\right) \setminus \tau(k^0)$. Then there exist neighbourhoods $U \subset \mathbb{R}$, $V \subset \mathbb{R}^d$ of λ_0, k^0 and a real-analytic function $h : U \times V \to \mathbb{R}$ satisfying*

1. *for all $\lambda \in U$, $k \in V$ one has $h(\lambda,k) = 0$ iff $0 \in \sigma\left(B^{(\sigma)}(\lambda,k)\right)$, and*
2. *for all $\lambda \in U$ one has $h(\lambda,.) \not\equiv 0$.*

Proof. We will construct an analytic extension of the operators $B^{(\sigma)}(\lambda,k)$ near $(\lambda,k)=(\lambda_0,k^0)$. (However now, in contrast to Subsection 3.3, with respect to all variables.) Indeed, since $\lambda_0\notin\tau(k^0)$, there exist neighbourhoods $\tilde U\subset\mathbb{C}$, $\tilde V\subset\mathbb{C}^d$ of λ_0, k^0 such that the functions β_n, $n\in\mathbb{Z}^d$, admit an analytic continuation to $\tilde U\times\tilde V$. Then we can define sectorial and closed forms $b^{(\sigma)}(z,\kappa)$ for $z\in\tilde U$, $\kappa\in\tilde V$ by (3.1) and obtain corresponding m-sectorial operators $B^{(\sigma)}(z,\kappa)$. These operators have compact resolvent and it is well-known that (after possibly decreasing $\tilde U$ and $\tilde V$) there is an analytic function $h:\tilde U\times\tilde V\to\mathbb{C}$ such that $h(z,\kappa)=0$ iff $0\in\sigma\left(B^{(\sigma)}(z,\kappa)\right)$. (Indeed, choosing h as a (regularized) determinant of $B^{(\sigma)}(z,\kappa)$ we see that $h(\lambda,k)\in\mathbb{R}$ if $\lambda\in U:=\tilde U\cap\mathbb{R}$, $k\in V:=\tilde V\cap\mathbb{R}^d$.) This proves property 1 in the proposition.
To prove property 2 we assume that $h(\lambda,.)\equiv 0$ for some $\lambda\in U$. We choose $k\in V$ such that $k_1\neq 0$ and $\lambda\notin\tau(k)$ and consider the family $B^{(\sigma)}(\lambda,\mu e_1+k')$, $\mu\in W$, constructed in Subsection 3.3. It follows from the Analytic Fredholm Alternative (see, e.g., Theorem VII.1.10 in [K]) that all operators of this family have 0 as an eigenvalue. But this contradicts Proposition 3.5. □

Finally, we can give the

Proof of Proposition 1.10. In order to cover threshold eigenvalues we include the functions h_n, $n\in\mathbb{Z}^d$, defined by $h_n(\lambda,k):=\sum_{j=1}^d(n_j+k_j)^2-\lambda$ in our collection. In the remaining set $\{(\lambda,k)\in\mathbb{R}\times Q^d:\lambda\notin\tau(k)\}$ we apply Proposition 3.7 noting that $0\in\sigma\left(B^{(\sigma)}(\lambda,k)\right)$ whenever $\lambda\in\sigma_p\left(H^{(\sigma)}(k)\right)$ by Proposition 3.1. □

4. Additional channels of scattering of the operators $H^{(\sigma)}$

4.1. **The negative spectrum of $H^{(\sigma)}$.** For $k\in Q^d$ we denote by $l(k)$ the number of eigenvalues of $H^{(\sigma)}(k)$ in $(-\infty,|k|^2)$, counting multiplicities. By Theorem 1.9 $l(k)$ is a finite number, possibly equal to 0. Moreover, let

$$\lambda_1(k)\leq\lambda_2(k)\leq\cdots\lambda_{l(k)}(k)<|k|^2 \tag{4.1}$$

the corresponding eigenvalues and set $\lambda_l(k):=|k|^2$ if $l>l(k)$. The functions λ_l are (Lipschitz) continuous on Q^d for each $l\in\mathbb{N}$. Combining this with (1.12) we find

$$\sigma\left(H^{(\sigma)}\right)=\bigcup_{l\in\mathbb{N}}\lambda_l(Q^d)\cup[0,+\infty), \tag{4.2}$$

i.e., the spectrum of $H^{(\sigma)}$ has band structure.
Under assumption (1.7) none of the functions λ_l is constant, since this would correspond to an eigenvalue of $H^{(\sigma)}$ contradicting Theorem 1.4.
If σ is non-negative, we have of course $\sigma\left(H^{(\sigma)}\right)\cap(-\infty,0)=\emptyset$. Conversely, we prove now that additional bands in the negative spectrum of $H^{(\sigma)}$ appear if σ is "non-positive in mean".

Proposition 4.1. *Assume that σ satisfies* (1.1) *and $\int_{\mathbb{T}^d} \sigma(x)\,dx \le 0$, $\sigma \not\equiv 0$. Then*

$$\sigma\left(H^{(\sigma)}\right) \cap (-\infty, 0) \neq \emptyset.$$

Proof. Indeed, fix $k \in Q^d$. We claim that under the above assumption $H^{(\sigma)}(k)$ has an eigenvalue smaller than $|k|^2$. We give the proof here only for the case $\int_{\mathbb{T}^d} \sigma(x)\,dx = 0$ the other one being simpler. (One can take then $\gamma = 0$ below, see [FrSh].) By our assumptions there exists $f \in H^1(\mathbb{T}^d)$ such that

$$\operatorname{Re} \int_{\mathbb{T}^d} \sigma(x) f(x)\,dx < 0, \qquad \int_{\mathbb{T}^d} f(x)\,dx = 0,$$

and we consider the "trial function"

$$u(x,y) := \frac{1}{(2\pi)^{d/2}} e^{-\alpha y} + \gamma f(x) e^{-\beta y}, \qquad (x,y) \in \Pi,$$

with constants $\alpha, \beta, \gamma > 0$ to be determined later. A simple calculation shows that

$$\frac{h^{(\sigma)}(k)[u]}{\|u\|^2} = |k|^2 + \frac{\alpha}{\beta + \alpha\gamma^2\|f\|^2}(I(\beta,\gamma) + \alpha\beta)$$

where

$$\begin{aligned} I(\beta,\gamma) := 2\beta\gamma \left(\tfrac{1}{(2\pi)^{d/2}} 2 \operatorname{Re} \int_{\mathbb{T}^d} \sigma(x) f(x)\,dx + \gamma \int_{\mathbb{T}^d} \sigma(x)|f(x)|^2\,dx \right) + \\ + \beta^2\gamma^2\|f\|^2 + \gamma^2\left(\|(D_x + k)f\|^2 - |k|^2\|f\|^2\right). \end{aligned}$$

By the variational principle our claim follows if we can prove that $I(\beta,\gamma) < 0$ for some $\beta, \gamma > 0$. This can be shown by minimizing $I(\beta,\gamma)$ with respect to β and then choosing γ small. □

Remark 4.2. The result of the proposition is sharp. Indeed, with more elaborate techniques one can show that if $\int_{\mathbb{T}^d} \sigma(x)\,dx > 0$ and $k \in (-\pi,\pi)^d$ there exists an $\alpha(k,\sigma) > 0$ such that $H^{(\alpha\sigma)}(k)$ has no eigenvalue below $|k|^2$ for $0 \le \alpha < \alpha(k,\sigma)$.

Finally, we remark that it is possible to construct examples where $H^{(\sigma)}$ has an arbitrary finite number of open gaps in its spectrum (see [FrSh] for the case of one open gap if $d = 1$).

4.2. **Surface states.** It is illuminating to look at the additional bands in the spectrum of $H^{(\sigma)}$ from the point of view of scattering theory. We recall that

$$\begin{aligned} \mathcal{R}(W_\pm^{(\sigma)}) &= \mathcal{U}^* \left(\int_{Q^d} \oplus \mathcal{R}(P_{ac}^{(\sigma)}(k))\,dk \right) \mathcal{U}, \\ \mathcal{R}(W_\pm^{(\sigma)})^\perp &= \mathcal{U}^* \left(\int_{Q^d} \oplus \mathcal{R}(P_p^{(\sigma)}(k))\,dk \right) \mathcal{U}, \end{aligned} \tag{4.3}$$

where $P_{ac}^{(\sigma)}(k)$, $P_p^{(\sigma)}(k)$ denote the projections onto the absolutely continuous and pure point subspaces of $H^{(\sigma)}(k)$, respectively. The first identity was established in the proof of Theorem 1.3, and the second one follows since $H^{(\sigma)}(k)$ has no singlar continuous spectrum by Theorem 1.8.

It is a general fact that the subspace $\mathcal{R}(W_\pm^{(\sigma)})$ reduces $H^{(\sigma)}$ and that the part of $H^{(\sigma)}$ on this subspace is unitarily equivalent to $H^{(0)}$. Additional bands in the spectrum of $H^{(\sigma)}$ are due to its part on $\mathcal{R}(W_\pm^{(\sigma)})^\perp$. We remark that the spectrum of that part might be *strictly* larger than $\bigcup_{l\in\mathbb{N}} \lambda_l(Q^d)$ in (4.2). This is because of possible embedded eigenvalues of the fiber operators $H^{(\sigma)}(k)$, see Examples 3.3.

From (4.3) we obtain easily (see [DaSi]) a geometric characterization of the spaces $\mathcal{R}(W_\pm^{(\sigma)})$, $\mathcal{R}(W_\pm^{(\sigma)})^\perp$. Namely, with the notation $U^{(\sigma)}(t) := \exp(-itH^{(\sigma)})$, $t \in \mathbb{R}$, one has

$$\mathcal{R}(W_\pm^{(\sigma)}) = \{u \in L_2(\mathbb{R}_+^{d+1}) : \lim_{t\to\pm\infty} \int_{\mathbb{R}^d\times(0,a)} |U^{(\sigma)}(t)u|^2\, dxdy = 0,\ a \in \mathbb{R}_+\},$$

$$\mathcal{R}(W_\pm^{(\sigma)})^\perp = \{u \in L_2(\mathbb{R}_+^{d+1}) : \lim_{a\to+\infty} \sup_{t\in\mathbb{R}} \int_{\mathbb{R}^d\times(a,+\infty)} |U^{(\sigma)}(t)u|^2\, dxdy = 0\}.$$

The second identity shows that states in $\mathcal{R}(W_\pm^{(\sigma)})^\perp$ are *surface states*, i.e., they are concentrated near the boundary for all time.

We have not been able to exclude the existence of bound states corresponding to eigenvalues of $H^{(\sigma)}$ under the assumption (1.1). However, under the assumption (1.7) the spectrum of $H^{(\sigma)}$ is absolutely continuous and $\mathcal{R}(W_\pm^{(\sigma)})^\perp$ represents *additional channels of scattering*. The appearance of additional channels of scattering is equivalent to the non-completeness of the wave operators $W_\pm^{(\sigma)}$. In Proposition 4.1 and Theorem 1.5 we gave sufficient conditions for the existence and non-existence of additional channels.

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