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Some aspects of the Floquet theory for the heat equation in a periodic domain

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Abstract. We treat the linear heat equation in a periodic waveguide $\Pi \subset \mathbb{R}^d$, with a regular enough boundary, by using the Floquet transform methods. Applying the Floquet transform F to the equation yields a heat equation with mixed boundary conditions on the periodic cell ϖ of Π, and we analyse the connection between the solutions of the two problems. The considerations involve a description of the spectral projections onto subspaces $\mathcal{H}_S \subset L^2(\Pi)$ corresponding certain spectral components. We also show that the translated Wannier functions form an orthonormal basis in $\mathcal{H}_S$.

1. Introduction

We consider the boundary-initial value problem for the classical linear heat equation with an unknown function u depending on place x and time t,

$$\partial_t u(x,t) = \Delta u(x,t), \quad (x,t) = (x_1, \dots, , x_d, t) \in \Pi \times \mathbb{R}^+ := \Pi \times (0,\infty), \tag{1.1}$$

$$u(x,0) = g(x), \quad x \in \Pi, \tag{1.2}$$

$$\partial_\nu^t u(x,t) = 0, \quad x \in \partial\Pi, \tag{1.3}$$

in a periodic, regular enough (see below) x-domain $\Pi \subset \mathbb{R}^d$, $d = 3, 4, 5 \dots$, which is contained in a cylinder with a bounded cross-section and axis in the x_1-direction. Here g is the given initial data, on which we assume that

$$\sum_{j=-\infty}^{\infty} \sup_{\substack{x \in \Pi, \\ j \le x_1 \le j+1}} |g(x)| < \infty \tag{1.4}$$

so that there holds $g \in L^\infty(\Pi) \cap L^1(\Pi) \subset L^2(\Pi)$. Moreover, $\partial_t = \partial/\partial t$ is the time-derivative, $\Delta = \nabla \cdot \nabla$ and ∇ is the gradient in the x-variable, ∂_ν is the outward

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normal derivative on the surface of a given x-domain and $\iota = 0$ or 1 so that in (1.3) we have the homogeneous Dirichlet or Neumann condition in the x-domain.

The main aim of this paper is to analyse the unique, classical solution $u = u(x, t)$ of the problem (1.1)–(1.3) by Floquet transform methods and in particular to relate the spectral representation of the solution with the eigenfunctions of the so called model problem (3.4)–(3.6) (see below), which is a spectral elliptic problem on the bounded periodic cell of Π.

We start by recalling some well-known facts on the solution u. First, all partial derivatives up to the first order in t and second order in x exist and are continuous functions of all variables. Moreover, u can be written by using the spectral representation of the elliptic (unbounded, self-adjoint, positive) operator $\mathcal{T}$, which is defined in a subdomain of $L^2(\Pi)$ ([5,40], Theorem VIII.6; [41], Theorem 13.30):

$$u(\cdot, t) = \int_\sigma e^{-\lambda t} dE_\lambda g = e^{\mathcal{T} t} g \ \text{ with } \mathcal{T} f = \int_\sigma \lambda dE_\lambda. \tag{1.5}$$

Here $\sigma = \sigma(\mathcal{T}) \subset [0, \infty)$ is the spectrum of $\mathcal{T}$, $(E_\lambda)_{\lambda \in [0,\infty)}$ is the resolution of the identity (see (3.14) of [45]), or the spectral family, associated with the spectral measure $P(\Omega)$ of $\mathcal{T}$, where $\Omega \subset \sigma$ is measurable (see the spectral theorem, e.g. Theorem 3.6. in [45], or Theorem VIII.6 of [40]), i.e. $E_\lambda = P((-\infty, \lambda])$. Formula (1.5) shows, among other things that we have

$$\lim_{t \to 0^+} u(, \cdot t) = g \ \text{ in the space } L^2(\Pi). \tag{1.6}$$

The elliptic problem related to (1.1)–(1.3) is the Laplace-Dirichlet or Neumann spectral problem (2.6)–(2.7) (see below) which is a standard spectral problem for the operator $\mathcal{T}$ in $L^2(\Pi)$. Our assumptions will include that the spectrum σ coincides with the essential $\sigma_{\text{ess}} = \sigma_{\text{ess}}(\mathcal{T})$ or continuous spectra of $\mathcal{T}$ and has band-gap structure (cf. Theorem 3.2), which is a consequence of the Floquet transform theory. The application of the Floquet transform F to the elliptic problem (2.6)–(2.7) leads to a spectral problem which depends on the Floquet parameter $\eta \in [-\pi, \pi]$, in a bounded periodic cell. The problem has a discrete spectrum consisting of a sequence of eigenvalues $\Lambda_k(\eta)$, $k \in \mathbb{N} = \{1, 2, 3, \ldots\}$, corresponding to an orthonormal sequence of eigenfunctions $V_k(\cdot; \eta)$. The general spectral band formula, see (3.18) below, shows that the spectral bands of σ emerge from the unions of the sets of eigenvalues $\Lambda_k(\eta)$.

The Floquet transform F is applied in Sect. 5 also directly to the original initial-boundary value problem (1.1)–(1.3), and the resulting description of the solution u is given in formula (5.11) of Proposition 5.1. In Sect. 6 we describe the heat semi-group and the spectral measure and projections of the operator $\mathcal{T}$ in terms of the eigenfunctions V_k of the model problem, see Theorems 6.3 and 6.5.

In Sect. 6 we consider a spectral subspace $\mathcal{H}_S$ corresponding to a disjoint component of σ. Since the related spectral bands do not overlap in this case, the presentation of the spectral projection corresponding to $\mathcal{H}_S$ in Theorem 6.5 can be simplified, see Proposition 7.1. Moreover, in Theorem 7.2 an orthonormal basis of $\mathcal{H}_S$: it is formed by certain inverse Floquet transforms $\mathsf{F}^{-1} V_k$ of the eigenfunctions and their translates (these are analogous to the so called Wannier functions, see the next paragraph). The consequences of these considerations to long time decay estimates of the parabolic problem are straightforward, as mentioned at the end of the paper. On the other hand, the exponentially decaying factor $e^{-\lambda t}$, cf. (1.5), which is characteristic for the solutions of the heat equation, is essential for our calculations and treatment of the spectral projections.

As for literature, we mention that band-gap spectra in geometric situations similar to ours have been considered e.g. in the papers [3,4,36,37]. However, the authors do not know papers dealing with the consequences of these studies to parabolic initial-boundary value problems. (Floquet-theory in the setting of parabolic equations has been studied e.g. in [19,23,24,30] and others, but these works concern periodicity with respect to the time-variable, which is unrelated to periodicity in the x-domain studied in the present work.) We also mention the following references as an incomplete list of other literature on the subject of spectral gaps in elliptic boundary value problems of various types: [2,7,8,10–13,15,17,18,31–34,47,48]. For presentations of the theory of Floquet transform, see [24], [26], [35]. In the setting of the time-independent Schrödinger equation with periodic potential, the functions corresponding to $\mathsf{F}^{-1} V_k$ are known as Wannier functions. For example the papers [22,25,38,39] contain studies of the question, whether the spectral subspace corresponding to a spectral band of the Schrödinger equation has an orthonormal basis spanned by translates of exponentially decreasing Wannier functions. See also [25] for more references especially to the literature on molecular chemistry.

As for the notation used in this article, $B(a, r)$ or $B_d(a, r)$ denote a Euclidean ball in $\mathbb{R}^d$ with center a and radius $r > 0$. For a measurable set $A \subset \mathbb{R}^d$, $|A|$ means the volume, and if $x \in \mathbb{R}^d$, then $\mathrm{dist}\,(x, A)$ denotes the Euclidean distance of x from the set A. By C, C', C_1 etc. (respectively, C_k, C'_η etc.) we denote generic positive constants which do not depend on the functions or variables in the calculations in question (resp. depend only on k, η) and the exact value of which may change from place to place. We write $\mathbb{N} = \{1, 2, 3, \ldots\}$, $\mathbb{Z} = \{0, \pm 1, \pm 2, \}$, $\mathbb{R}_+ = (0, \infty)$. If $x \in \mathbb{R}$, $[x]$ stands for the largest integer not larger than x. Given $x = (x_1, x') \in \mathbb{R} \times \mathbb{R}^{d-1}$, we write $x^{\mathrm{tr}} = (x_1 - [x_1], x')$. For $j \in \mathbb{N}$ we denote $\partial_j := \partial/\partial x_j$. Moreover, given a domain $\Omega \subset \mathbb{R}^d$, we denote by $\|u\|_\Omega$ and $(u, v)_\Omega$ the norm and scalar product of the space $L^2(\Omega)$ with the complex scalar field. The notation for the other $L^p(\Omega)$-spaces is standard. In general, given a Banach space X, its norm is denoted by $\|\cdot\|_X$. The standard Sobolev-Hilbert space of order $k \in \mathbb{N}$ is denoted by $H^k(\Omega)$, and $H^k_0(\Omega)$ is its closed subspace spanned by the compactly supported infinitely smooth test functions, i.e., elements of the space $C_0^\infty(\Omega)$. Moreover, $C_B(\Omega)$ (respectively, $C_B^1(\Omega)$) denotes the space of bounded, continuous functions on Ω (resp. continuously differentiable functions on Ω with bounded partial derivatives of the first order). The Hilbert space of square summable sequences of complex numbers is denoted by ℓ^2, or by $\ell^2(\mathbb{N})$ or $\ell^2(\mathbb{Z})$, if it is necessary to indicate the index set.

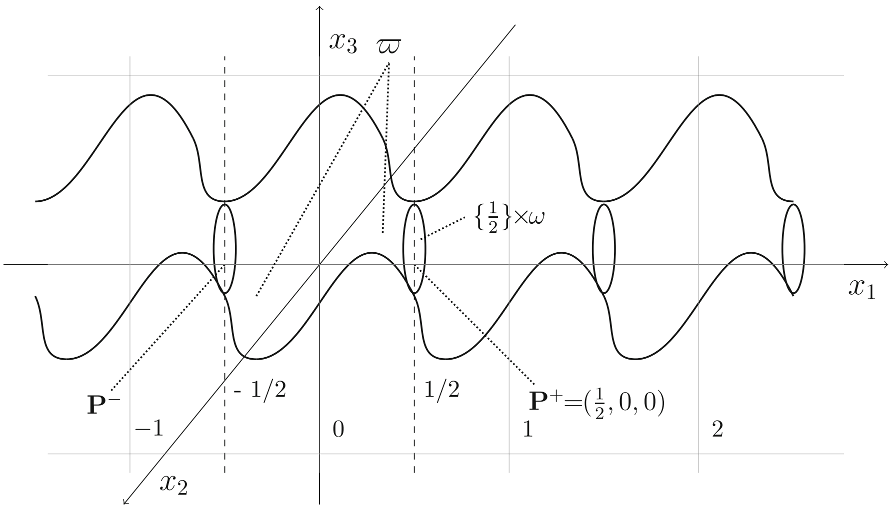

Figure 1. Periodic domain $\Pi \subset \mathbb{R}^3$

We will need to pay attention to some details of Banach-space valued integrals. For the basic theory of vector valued L^2-spaces and the Bochner-integral we refer to [20] (Fig. 1).

2. Preliminaries

Let us proceed with the details of the geometric assumptions. By $\varpi \subset \mathbb{R}^d$ we denote the primary periodic cell

$$\varpi \subset \{x = (x_1, x') \in \mathbb{R} \times \mathbb{R}^{d-1}, |x_1| < 1/2\}, \tag{2.1}$$

which is a bounded domain in $\mathbb{R}^d$ with boundary $\partial\varpi$. We write $T^\pm = \{x \in \mathbb{R}^d : x_1 = \pm 1/2\}$ and $P^\pm = (\pm 1/2, 0, \dots, 0) \in T^\pm$ and assume that there holds

$$\partial\varpi \cap T^\pm = \{\pm 1/2\} \times \overline{\omega} \tag{2.2}$$

for some open set $\omega \subset \mathbb{R}^{d-1}$ containing the origin of $(0, \dots, 0)$ of $\mathbb{R}^{d-1}$ (hence, $P^\pm \subset \partial\varpi$). Furthermore, we denote the translates of ϖ by

$$\varpi(j) := \{x : (x_1 - j, x') \in \varpi\} \;\; j \in \mathbb{Z}, \tag{2.3}$$

and define the main periodic domain (waveguide) Π as the interior of the union

$$\bigcup_{j \in \mathbb{Z}} \overline{\varpi(j)}. \tag{2.4}$$

Assumption 1. We require that the boundary $\partial\Pi$ is of smoothness C^κ, where $\kappa \in \mathbb{N}$ is the smallest integer such that

$$\kappa > \frac{d}{2} + \frac{3}{2}. \tag{2.5}$$

We will consider the following spectral Laplace-Dirichlet or Neumann problem for an unknown function v on the domain Π, related with the initial-boundary value problem (1.1)–(1.3):

$$-\Delta v(x) = \lambda v(x), \quad x \in \Pi, \tag{2.6}$$

$$\partial_\nu^\iota v(x) = 0, \quad x \in \partial\Pi, \quad \iota = 0 \text{ or } 1. \tag{2.7}$$

The variational formulation of this problem, see [28,29], reads in the Neumann case $\iota = 1$ as

$$(\nabla u, \nabla v)_\Pi = \lambda (u, v)_\Pi \quad v \in H^1(\Pi), \tag{2.8}$$

and in the Dirichlet case $\iota = 0$ the space $H^1(\Pi)$ is replaced by $H_0^1(\Pi)$. Also, the negative Laplacian $-\Delta$ defines an unbounded self–adjoint positive operator $\mathcal{T} : \mathcal{D} \to L^2(\Pi)$ with the domain of definition $\mathcal{D} = H_0^1(\Pi) \cap H^2(\Pi)$ in the Dirichlet case or $\mathcal{D} = H_\bullet^1(\Pi) \cap H^2(\Pi)$ in the Neumann case, where

$$H_\bullet^1(\Pi) = \{f \in H^1(\Pi) \, : \, \partial_\nu f(x) = 0 \text{ for almost all } x \in \partial\Pi\}. \tag{2.9}$$

By positivity, the spectrum $\sigma = \sigma(\mathcal{T})$ (the same as the spectrum of the problem (2.6)–(2.7)) lies in $\overline{\mathbb{R}}_+ = [0, \infty)$, and since the embedding $H^1(\Pi) \subset L^2(\Pi)$ is not compact in the unbounded domain Π, the essential spectrum $\sigma_{\text{ess}} = \sigma_{\text{ess}}(\mathcal{T})$ is not empty (cf. [5, Th.10.1.5]). Actually, it is a well known consequence of the Floquet transform theory, that the spectrum has the so called band-gap structure. We will recall this in Sect. 3, and we later use this to derive consequences on the long-time asymptotics of the solutions of the problem (1.1)–(1.3).

Actually, we pose the following

Assumption 2. The spectrum σ is absolutely continuous.

This assumption in particular implies that $\sigma(\mathcal{T}) = \sigma_{\text{ess}}(\mathcal{T})$ and that, for the problem (2.6)–(2.7), there does not exist eigenvalues of finite or infinite multiplicity (with eigenfunctions belonging to $L^2(\Pi)$. It is generally believed that indeed σ is absolutely continuous in the situation of this paper, although this has not yet been proved. For example, by the result of [14], the absolute continuity holds, if the boundary $\partial\Pi$ is smooth and in addition ϖ and thus Π are symmetric under the reflection $x_1 \mapsto -x_1$. Partial positive results on the absolute continuity can also be found e.g. [9,24,27,42–44]; see also the references on p. 383 of [26].

3. Floquet transform and band–gap spectrum of the elliptic problem

In this section we recall the basics of the Floquet transform theory and apply it in order to turn problem (2.6)–(2.7) into a model problem in the periodic cell ϖ. The well-known Theorem 3.2 recalls how the band-gap structure of the spectrum of $\mathcal{T}$ emerges from the spectra of the model problems.

We recall the definition of the Floquet transform (see for example [16,24,26,35]):

$$\mathsf{F} : v(x) \mapsto V(x;\eta) = \frac{1}{\sqrt{2\pi}} \sum_{m\in\mathbb{Z}} \exp(-i\eta m) v(x_1 + m, x'), \tag{3.1}$$

where $v \in L^2(\Pi)$, $x = (x_1, x') \in \Pi$ on the left, $\eta \in [-\pi, \pi]$, and $x \in \varpi$ on the right. This operator is a linear isometry from $L^2(\Pi)$ onto $L^2(-\pi, \pi; L^2(\varpi))$, which also preserves the inner product; the inner product of $L^2(-\pi, \pi; L^2(\varpi)) \ni f, g$ is defined by

$$(f, g)_{L^2(-\pi,\pi;L^2(\varpi))} = \int_{-\pi}^{\pi} \big(f(\cdot;\eta), g(\cdot;\eta)\big)_{\varpi} d\eta. \tag{3.2}$$

Moreover, it is a (Banach-space) isomorphism from $H^1(\Pi)$ onto $L^2(-\pi, \pi; H^1_\eta(\varpi))$ (see e.g. [26, Th. 4.2, Th. 4.8], [35, § 3.4], [31, Cor. 3.4.3]). Here $L^2(-\pi, \pi; L^2(\varpi))$ consists of (complex) $L^2(\varpi)$–valued functions on the interval $[-\pi, \pi]$, which are L^2-integrable in the sense of Bochner, and the space $L^2(-\pi, \pi; H^1_\eta(\varpi))$ is the closed subspace of $L^2(-\pi, \pi; H^1(\varpi))$ consisting of such vector valued functions f that $f(\cdot;\eta) \in H^1_\eta(\varpi)$ for almost all η. Moreover, $H^1_\eta(\varpi)$ is the subspace of $H^1(\varpi)$ consisting of functions that satisfy, in the sense of traces, the quasiperiodic boundary condition which is the first equation in (3.6), below. The inverse transform has the formula

$$\mathsf{F}^{-1} g(x) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{i[x_1]\eta} g(x^{\mathrm{tr}};\eta) d\eta, \tag{3.3}$$

where $x \in \Pi$, $g \in L^2(-\pi, \pi; L^2(\varpi))$, and $x^{\mathrm{tr}} = (x_1 - [x_1], x')$ so that $x^{\mathrm{tr}} \in \varpi$ for all $x \in \Pi$.

Using the Floquet transform, problem (2.6)–(2.7) turns into the following model spectral problem in the periodic cell ϖ, (2.1),

$$-\Delta V(x;\eta) = \Lambda(\eta) V(x;\eta), \quad x \in \varpi, \tag{3.4}$$

$$\partial_\nu^\iota V(x;\eta) = 0, x \in \partial\varpi \cap \partial\Pi, \quad \iota = 0 \text{ or } 1, \tag{3.5}$$

$$V\Big(\frac{1}{2}, x'\Big) = e^{i\eta} V\Big(-\frac{1}{2}, x'\Big), \ \partial_1 V\Big(\frac{1}{2}, x'\Big) = e^{i\eta} \partial_1 V\Big(-\frac{1}{2}, x'\Big), \ x' \in \omega, \tag{3.6}$$

where $\Lambda = \Lambda(\eta)$ is just a new notation for the spectral parameter. The variational formulation of the problem (3.4)–(3.6) in the case $\iota = 1$ is to find $V = V(\cdot;\eta) \in H^1_\eta(\varpi)$, $V \neq 0$, and Λ such that

$$\big(\nabla V, \nabla U\big)_\varpi = \Lambda (V, U)_\varpi, \tag{3.7}$$

for all $U \in H^1_\eta(\varpi)$; the inner product is that of $L^2(\varpi)$. The case $\iota = 0$ is similar, except that in (3.7) the space $H^1_\eta(\varpi)$ is replaced by its closed subspace $H^1_{0,\eta}(\varpi)$, which consists of functions vanishing on the boundary $\partial\varpi \cap \partial\Pi$. In a standard way we also define, for every $\eta \in [-\pi, \pi]$, an unbounded, self-adjoint, positive operator $S = S(\eta) : \mathcal{D}_\eta \to L^2(\varpi)$ such that problem (3.4)–(3.6) is equivalent to the equation $S(\eta)V = \Lambda V$. We will not need to specify the domains $\mathcal{D}_\eta \subset L^2(\varpi)$ precisely, but in the Neumann case $\iota = 1$ we will need the sesquilinear, lower semibounded form associated with $S(\eta)$, which is the mapping

$$A_\eta : H^1_\eta(\varpi) \times H^1_\eta(\varpi) \to \mathbb{C}, \quad A_\eta(V, U) = \big(\nabla V, \nabla U\big)_\varpi, \tag{3.8}$$

see e.g. [5], Section 10.1–2. Since the domain ϖ is bounded, the embedding $H^1_\eta(\varpi) \subset L^2(\varpi)$ is compact and the spectra of the problem in both cases $\iota = 0, 1$ are discrete, see [5], Th. 10.1.5. The numbers

$$0 \le \Lambda_1(\eta) \le \Lambda_2(\eta) \le \cdots \le \Lambda_p(\eta) \le \cdots \to +\infty, \tag{3.9}$$

form the sequence of eigenvalues (counting multiplicities) for the model problem, and the corresponding eigenvectors are denoted by $V_k = V_k(\cdot;\eta) \in H^1_\eta(\varpi)$, $k \in \mathbb{N}$. We require the orthogonality and normalization conditions

$$(V_k, V_\ell)_\varpi = \delta_{k,\ell} \;\; k, \ell = 1, 2, \ldots, \tag{3.10}$$

so that for any fixed $\eta \in [-\pi, \pi]$ the functions $V_k(\cdot;\eta)$, $k \in \mathbb{N}$, form an orthonormal basis of $L^2(\varpi)$.

Remark 3.1. Let us derive some Sobolev- and sup-norm estimates for the eigenfunctions V_k. Let $B \subset (-1/2, 1/2) \times \mathbb{R}^{d-1} \subset \mathbb{R}^d$ be a ball such that $B \cap \varpi \neq \emptyset$ and $B \cap T^\pm = \emptyset$. Then, an eigenfunction V_k satisfies

$$-\Delta V_k = \Lambda_k V_k \quad \text{in } \Pi \cap B \tag{3.11}$$

$$\partial_\nu^\iota V_k = 0 \quad \text{on } \Gamma = \partial\Pi \cap \partial\varpi \cap \overline{B}. \tag{3.12}$$

Also, according to Assumption 1, the boundary Γ is of smoothness C^κ, $\kappa > d/2+3/2$, hence, we can apply the local elliptic estimate in Theorem 15.2 in [1] to get

$$\|V_k\|_{H^\ell(\Pi\cap B)} \le C\big(\|\Lambda_k V_k\|_{H^{\ell-2}(\Pi\cap B)} + \|V_k\|_{\Pi\cap B}\big) \tag{3.13}$$

for all $\ell = 2, 3, \ldots, \kappa$. Thus, (3.10) and (3.13) directly yield a bound for the H^2-norm of V_k, which can be used a second time with $\ell = 4$ to obtain an estimate for the H^4-norm of V_k. Repeating this procedure, if necessary, one finally obtains

$$\|V_k\|_{H^\kappa(\Pi\cap B)} \le C(\Lambda_k + 1)^{d^*} \tag{3.14}$$

for some integer d^* depending on d (to be precise, $d^* = [d/4]+1$). Then, the Sobolev embedding $H^\kappa(\Pi \cap B) \hookrightarrow C^1_B(\Pi \cap B)$ (see 2.5) gives us

$$\|V_k\|_{L^\infty(\Pi\cap B)} + \|\nabla V_k\|_{L^\infty(\Pi\cap B)} \le C(\Lambda_k + 1)^{d^*}. \tag{3.15}$$

Note that the constants C both in (3.14) and (3.15) can be chosen independently of η or k.

The estimate (3.15) can also be shown for any ball $\widetilde{B} \subset (0,1) \times \mathbb{R}^{d-1} \subset \mathbb{R}^d$ with radius, say, at most $1/4$ and $\widetilde{B} \cap \varpi \neq \emptyset$ and $\widetilde{B} \cap T^+ \neq \emptyset$, by using the quasiperiodicity. Namely, we define the function

$$\widetilde{V}_k(x;\eta) = \begin{cases} V_k(x;\eta), & x \in \overline{\varpi},\ 0 < x_1 \le 1/2 \\ e^{i\eta} V_k(x-1;\eta), & x \in \overline{\varpi(1)},\ 1/2 < x_1 \le 1, \end{cases} \tag{3.16}$$

and observe (using (3.6) among other things) that this is an eigenfunction with eigenvalue $\Lambda_k(\eta)$ of a problem similar to (3.4)–(3.6), but in the cell $\widetilde{\varpi} = \Pi \cap (0,1) \times \mathbb{R}^{d-1}$ instead of ϖ. The previous argument applies and yields the same Hölder estimate for $\widetilde{V}_k$ and thus for V_k in the ball $\widetilde{B}$.

The balls with $B \cap T^- \neq \emptyset$ are treated in the same way. Since ϖ can be covered by finitely many balls B and $\widetilde{B}$, we can combine these estimates and deduce that every eigenfunction $V_k(\cdot;\eta)$ belongs to $H^\kappa(\varpi)$ and $C^1_B(\varpi)$, and

$$\begin{aligned} &\|V_k(\cdot;\eta)\|_{H^\kappa(\varpi)} \le C\Lambda_k^{d^*}, \\ &\|V_k(\cdot;\eta)\|_{L^\infty(\varpi)} + \|\nabla V_k(\cdot;\eta)\|_{L^\infty(\varpi)} \le C(\Lambda_k + 1)^{d^*} \end{aligned} \tag{3.17}$$

where d^* is as in (3.14) and the constant C in particular does not depend k or η.

For the following fact, see [35, Th. 3.4.6], [31, Th. 2.1], and [24,26] in the case of the operators in the entire Euclidean space.

Theorem 3.2. *A number λ belongs to the resolvent set or to the discrete spectrum of $\mathcal{T}$, if and only if it does not coincide with $\Lambda_k(\eta)$ for any $\eta \in [-\pi,\pi]$ and k.*

Hence, $\sigma_{\rm ess}(\mathcal{T})$ and thus also $\sigma(\mathcal{T})$ (see Assumption 2) get the band–gap structure, namely

$$\sigma_{\rm ess}(\mathcal{T}) = \bigcup_{k=1}^{\infty} \Upsilon_k, \tag{3.18}$$

where the kth spectral band is defined by

$$\Upsilon_k = \{\Lambda_k(\eta)\ \ \eta \in [-\pi,\pi]\}. \tag{3.19}$$

It is known that the functions $\mathbb{R} \ni \eta \mapsto \Lambda_k(\eta)$ are continuous and even piecewise real analytic (see [21, Ch.7]), which implies that every Υ_k is a closed interval, and 2π–periodic: replacing η by $\eta + 2\pi\ell$, the function $e^{-i2\pi\ell z} V_k$ is again an eigenfunction with eigenvalue $\Lambda_k(\eta)$, for all $\ell \in \mathbb{Z}$. We denote the endpoints of the spectral bands Υ_k, $k \in \mathbb{N}$, by

$$m_k = \min\{\Lambda_k(\eta) \,:\, \eta \in [-\pi, \pi]\}, \quad M_k = \max\{\Lambda_k(\eta) \,:\, \eta \in [-\pi, \pi]\}. \tag{3.20}$$

Remark 3.3. Our Assumption 2 implies that none of the functions $\eta \mapsto \Lambda_k(\eta)$ is constant (even on a subset of $[-\pi, \pi]$ with positive measure). Namely, if $\Lambda_k(\eta) = r$ for some number $r \in \mathbb{R}$ on a set of positive measure, then r is an eigenvalue of $\mathcal{T}$, which we are assuming not to happen. See Section 6.3. of [26].

4. Lower bounds for the eigenvalues of the model problem.

The aim of this section is to prove a lower bound for the eigenvalues (3.9) of the model problem. For the purposes of this paper, there is no need to approach optimal results, namely, quite rough estimates will suffice to guarantee that the series (5.8) converges well for all $t > 0$. The result we need is contained in the following lemma. In the Dirichlet case, the lower bound can be obtained by comparing the eigenvalues with those of the corresponding problem on a cube and using the max-min-principle. In the Neumann case it is possible to give a simpler proof with the help of associated semibounded forms and a comparison with the eigenvalues of the pure Neumann problem in ϖ.

Lemma 4.1. *There is a constant $\gamma > 0$ such that for all $k \in \mathbb{N}$, $\eta \in [-\pi, \pi]$, we have the lower bound*

$$\Lambda_k(\eta) \geq \gamma k^{2/d} \tag{4.1}$$

for the eigenvalues (3.9).

Proof. We first consider the Dirichlet case $\iota = 0$ and choose a large enough number $M > 0$ such that $\varpi \subset (-1/2, 1/2) \times (-M, M)^{d-1} =: Q_M$. We fix k and η and consider the following eigenvalue problem,

$$-\Delta \widetilde{V}(x;\eta) = \widetilde{\Lambda}(\eta)\widetilde{V}(x;\eta), \quad x \in Q_M, \tag{4.2}$$

$$\widetilde{V}(x;\eta) = 0, \quad x_1 \in (-1/2, 1/2), \ x_j = \pm M \text{ for } j = 2, \dots, d, \tag{4.3}$$

$$\begin{aligned} \widetilde{V}(1/2, x') &= e^{i\eta}\widetilde{V}(-1/2, x'), \\ \partial_1 \widetilde{V}(1/2, x') &= e^{i\eta}\partial_1 \widetilde{V}(-1/2, x'), \ x' \in [-M, M]^{d-1}. \end{aligned} \tag{4.4}$$

The variational formulation of this problem is composed in the same way as for the problem (3.4)–(3.6) and it amounts to finding $V \in H^1_{0,\eta}(Q_M)$ and Λ such that

$$(\nabla V, \nabla U)_{Q_M} = \Lambda(V, U)_{Q_M} \tag{4.5}$$

for all $U \in H^1_{0,\eta}(Q_M)$; this Sobolev-type space is defined in the same way as in Sect. 3. Also, the solution of the problem consists of an increasing, positive, unbounded sequence of eigenvalues $\widetilde{\Lambda}_k = \widetilde{\Lambda}_k(\eta)$ together with eigenfunctions, which are of the form

$$e^{i\eta(x_1-1/2)+i2\pi n_1 x_1} \prod_{j=2}^{d} \cos\Big(\frac{n_j \pi x_j}{2M}\Big), \tag{4.6}$$

where $n = (n_1, \ldots, n_d)$ is running over all multi-indices with $n_1 \geq 0$ and $n_j > 0$ for $j = 2, \ldots, d$. The function (4.6) corresponds to the eigenvalue $(\eta + 2\pi n_1)^2 + \pi^2(4M)^{-2}\sum_{j=2}^{d} n_j^2$, hence, given $k \in \mathbb{N}$, there are less than $C_M k^{d/2}$ such eigenvalues belonging to the interval $[0, k]$, where $C_M > 0$ is a large enough constant. We thus obtain the lower bound

$$\widetilde{\Lambda}_k(\eta) \geq Ck^{2/d} \tag{4.7}$$

for the kth eigenvalue of the problem (4.2)–(4.4).

On the other hand, the eigenvalue $\widetilde{\Lambda}_k(\eta)$ is obtained from the max-min-principle ([5,40], Theorem 10.2.2]) as

$$\widetilde{\Lambda}_k(\eta) = \sup_{H^{(k)}} \inf_{0 \neq U \in H^{(k)}} \frac{(\nabla U, \nabla U)_{Q_M}}{(U, U)_{Q_M}} \tag{4.8}$$

where in the supremum, $H^{(k)}$ is running over all $k-1$-codimensional subspaces of $H^1_{0,\eta}(Q_M)$. We now fix $k \in \mathbb{N}$ and extend all eigenfunctions $V_j(\cdot;\eta)$, $j = 1, \ldots, k$, as 0 to the domain Q_M and denote the extensions by $\widetilde{V}_j(\cdot;\eta)$. These functions belong to $H^1_{0,\eta}(Q_M)$ and still form an orthonormal sequence in $L^2(Q_M)$, by (3.10), and also an orthogonal sequence in $H^1_{0,\eta}(Q_M)$, by (3.7). Thus, given an arbitrary $k-1$-codimensional subspace $H^{(k)}$ of $H^1_{0,\eta}(\varpi)$, there are coefficients $\varrho_j \in \mathbb{C}$ such that

$$\sum_{j=1}^{k} \varrho_j \widetilde{V}_j(\cdot;\eta) \in H^{(k)} \quad \text{and} \quad \sum_{j=1}^{k} |\varrho_j|^2 = 1. \tag{4.9}$$

Given an arbitrary $\varepsilon > 0$ we choose a $k-1$-codimensional subspace $\mathbf{H}$ of $H^1_{0,\eta}(Q_M)$ such that

$$\sup_{H^{(k)}} \inf_{0 \neq U \in H^{(k)}} \frac{(\nabla U, \nabla U)_{Q_M}}{(U, U)_{Q_M}} \leq \inf_{0 \neq U \in \mathbf{H}} \frac{(\nabla U, \nabla U)_{Q_M}}{(U, U)_{Q_M}} + \varepsilon \tag{4.10}$$

and choose the coefficients ϱ_j such that (4.9) holds for $\mathbf{H}$. Noting that $(V_j, V_\ell)_\varpi = \Lambda_j \delta_{j,\ell}$ by (3.7), (3.10), we obtain from (4.8), (3.9), (4.10)

$$\begin{aligned}
\widetilde{\Lambda}_k(\eta) &\leq \frac{\Big(\sum_{j=1}^{k} \varrho_j \nabla \widetilde{V}_j(\cdot;\eta), \sum_{j=1}^{k} \varrho_j \nabla \widetilde{V}_j(\cdot;\eta)\Big)_{Q_M}}{\Big(\sum_{j=1}^{k} \varrho_j \widetilde{V}_j(\cdot;\eta), \sum_{j=1}^{k} \varrho_j \widetilde{V}_j(\cdot;\eta)\Big)_{Q_M}} + \varepsilon \\
&= \frac{\Big(\sum_{j=1}^{k} \varrho_j \nabla V_j(\cdot;\eta), \sum_{j=1}^{k} \varrho_j \nabla V_j(\cdot;\eta)\Big)_{\varpi}}{\Big(\sum_{j=1}^{k} \varrho_j V_j(\cdot;\eta), \sum_{j=1}^{k} \varrho_j V_j(\cdot;\eta)\Big)_{\varpi}} + \varepsilon
\end{aligned}$$

$$= \frac{\sum_{j=1}^{k} |\varrho_j|^2 \Lambda_j(\eta)}{\sum_{j=1}^{k} |\varrho_j|^2} + \varepsilon \leq \sum_{j=1}^{k} |\varrho_j|^2 \Lambda_k(\eta) + \varepsilon = \Lambda_k(\eta) + \varepsilon. \quad (4.11)$$

This and (4.7) imply (4.1) in the Dirichlet case for some constant $\gamma > 0$, since $\varepsilon > 0$ was arbitrary.

In the Neumann case $\iota = 1$ we consider the pure Neumann problem in the periodic cell,

$$-\widehat{\Delta} V(x) = \widehat{\Lambda}(\eta) V(x) \text{ for } x \in \varpi, \quad \partial_\nu \widehat{V}(x) = 0 \text{ for } x \in \partial\varpi. \quad (4.12)$$

Again, this problem has an unbounded, non-negative sequence of eigenvalues $0 = \widehat{\Lambda}_1 < \widehat{\Lambda}_2 \leq \widehat{\Lambda}_3 \leq \cdots$, for which there holds

$$\widehat{\Lambda}_k \geq C_\varpi k^{2/d}, \qquad k \geq 2, \quad (4.13)$$

for example just by the classical Weyl estimate [46]. Moreover, the standard problem operator of (4.12), denoted here by S_N, is associated with the sesquilinear, lower semibounded form

$$A_N : H^1(\varpi) \times H^1(\varpi) \to \mathbb{C}, \quad A_N(V, U) = (\nabla V, \nabla U)_\varpi. \quad (4.14)$$

Now, comparing with (3.8), there holds $S(\eta) > S_N$ in the sense of the discussion preceding Theorem 10.2.4. of [5]. This reference and (4.13) imply that we have

$$\Lambda_k(\eta) \geq \widehat{\Lambda}_k \geq C_\varpi k^{2/d}. \quad (4.15)$$

This proves the lemma.

5. Solution of the initial-boundary value problem via Floquet transform

Applying the Floquet transform formally with respect to the x_1-variable to the problem (1.1)–(1.3) leads to the following system for the function $U = \mathsf{F}u$:

$$\partial_t U(x, t; \eta) = \Delta U(x, t; \eta), \quad x \in \varpi,\ t > 0,\ \eta \in [-\pi, \pi] \quad (5.1)$$

$$U(x, 0; \eta) = G(x; \eta) := \mathsf{F}g(x; \eta), \quad x \in \varpi,\ \eta \in [-\pi, \pi] \quad (5.2)$$

$$\partial_\nu^\iota U(x, t; \eta) = 0, \quad x \in \partial\varpi \cap \partial\Pi,\ t > 0,\ \eta \in [-\pi, \pi] \quad (5.3)$$

$$\begin{aligned} U((1/2, x'), t; \eta) &= e^{i\eta} U((-1/2, x'), t; \eta) \text{ and} \\ \partial_1 U((1/2, x'), t; \eta) &= e^{i\eta} \partial_1 U((-1/2, x'), t; \eta), \quad x' \in \omega,\ t > 0,\ \eta \in [-\pi, \pi] \end{aligned} \quad (5.4)$$

where g is the Cauchy data in (1.2) and $\iota = 0$ (Dirichlet case) or 1 (Neumann case). Note that the assumption (1.4) and the very definition of the Floquet transform, (3.1) yield

$$\sup_{\substack{x \in \varpi, \\ \eta \in [-\pi, \pi]}} |G(x; \eta)| < \infty. \quad (5.5)$$

For a fixed η, (5.1)–(5.4) is an initial-boundary value problem for the heat equation in a bounded x-domain, although the mixed boundary conditions (5.3)–(5.4) for the unknown function U are somewhat unconventional. Yet, the corresponding spectral elliptic problem is nothing but (3.4)–(3.6), associated with the positive, self-adjoint operator $\mathcal{S} = \mathcal{S}(\eta)$ with domain $D_\eta \subset L^2(\varpi)$. The operators $\mathcal{S}$ are in particular maximal monotone, hence the Hille-Yosida-theorem ([6], Theorem 7.4) implies that problem (5.1)–(5.4) has a unique solution

$$U \in C^1\big([0,\infty); L^2(\varpi)\big) \cap C\big([0,\infty); D_\eta\big), \tag{5.6}$$

and we moreover have

$$\|U(\cdot,t;\eta)\|_{L^2(\varpi)} \le \|G(\cdot;\eta)\|_{L^2(\varpi)} \tag{5.7}$$

for every η.

We will show shortly that the following series coincides with (5.6):

$$U(x,t;\eta) = \sum_{k=1}^{\infty} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x;\eta). \tag{5.8}$$

Here,

$$G_k(\eta) = \big(G(\cdot;\eta), V_k(\cdot;\eta)\big)_\varpi = \big((\mathsf{F}g)(\cdot;\eta), V_k(\cdot;\eta)\big)_\varpi \tag{5.9}$$

are the coordinates of the initial data $G(\cdot;\eta)$ in the orthonormal basis $\big(V_k(\cdot;\eta)\big)_{k=1}^\infty$ of $L^2(\varpi)$. Thus, for all η and $t \ge 0$, (5.8) converges in $L^2(\varpi)$, and the sequence $\big(G_k(\eta)\big)_{k=1}^\infty$ belongs to ℓ^2. Note that due to (5.5) and the normalization (3.10), there exists a constant $C > 0$ such that

$$|G_k(\eta)| \le C \tag{5.10}$$

for all $k \in \mathbb{N}$ and $\eta \in [-\pi,\pi]$.

Moreover, if $t > 0$, then Lemma 4.1 implies that the series (5.8) together with its termwise t-derivative converge uniformly with respect to t and x. Thus, termwise differentiation yields the function $\partial_t U$. Similarly, termwise differentiation with Δ yields $-\Delta U$, since the terms of the series contain eigenfunctions of Δ and the resulting coefficients $\Lambda_k(\eta)e^{-\Lambda_k(\eta)t}$ are still small enough. We obtain that the series (5.8) is a solution of (5.1).

As for the boundary conditions (5.3)–(5.4), we obtain by (3.17) and Lemma 4.1 that the series (5.8) converges absolutely also in $H^\kappa(\varpi)$ for every $t > 0$, hence, these boundary conditions are satisfied by the sum of the series, since this is true for all terms.

Finally, (5.2) holds since due to the orthonormality of the functions V_k we have for U of the series (5.8)

$$\lim_{t\to 0^+} U(\cdot,t;\eta) = \sum_{k=1}^{\infty} G_k(\eta) V_k(\cdot;\eta) = G(\cdot;\eta)$$

as a limit in the space $L^2(\varpi)$, for every η. Since the solution of (5.1)–(5.4) is unique, (5.6) and (5.8) coincide.

We next verify that $\mathsf{F}^{-1}U$ is the unique solution of the original initial-boundary problem (1.1)–(1.3). Indeed, by (5.6), (5.7) and (5.5), the function $\partial_t U(\cdot, t; \eta)$ (respectively, due to (5.1), also $\Delta U(\cdot, t; \eta)$) belong to $L^2(\varpi)$ for every $t \geq 0$ and η, with an η-uniform bound for its norm in $L^2(\varpi)$. By the Banach-space valued Lebesgue dominated convergence theorem, e.g. Proposition 1.2.5 in [20], and just the integral definition of the inverse Floquet transform, this implies that the derivative ∂_t (respectively, Δ) and F^{-1} can be commuted. We obtain that $\mathsf{F}^{-1}U$ satisfies (1.1). As a consequence of (5.3), it also satisfies the boundary condition (1.2). Finally, by (5.6), $U(, t; \eta) \to G(\cdot; \eta)$ in $L^2(\varpi)$ as $t \to 0^+$ for every η, hence $\mathsf{F}^{-1}U(\cdot, t) \to g$ again by the vector valued Lebesgue theorem. Hence, also the initial condition (1.3) holds, which completes the proof of the claim.

Proposition 5.1. *The unique solution u of the problem* (1.1)–(1.3) *can be written for* $t > 0$ *as the series*

$$\begin{aligned} u(x,t) &= \sum_{k=1}^{\infty} \mathsf{F}^{-1} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(\cdot; \eta) \\ &= \frac{1}{\sqrt{2\pi}} \sum_{k=1}^{\infty} \int_{-\pi}^{\pi} e^{i[x_1]\eta} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x^{\mathrm{tr}}; \eta) d\eta, \end{aligned} \tag{5.11}$$

which converges absolutely in $L^2(\Pi)$. *Here,* G_k *is as in (5.9) and* V_k *is the kth eigenfunction in (3.10).*

Proof. As a consequence of (3.10) and Lemma 4.1, the series (5.8) converges in $L^2(\varpi)$ absolutely and uniformly with respect to η, hence it converges absolutely in $L^2(-\pi, \pi; L^2(\varpi))$. The absolute convergence of the series (5.11) in $L^2(\Pi)$ thus follows from the continuity of the operator F^{-1} in the relevant Hilbert spaces. Hence, (5.11) coincides with $\mathsf{F}^{-1}U$, which by the argument above is the unique solution of (1.1)–(1.3). $\square$

6. Spectral projections: general formulas

In this section we present the main general results concerning the presentation of the spectral projections $P(\Omega)$ of the operator $\mathcal{T}$, see (1.5) in terms of the eigenfunctions V_k of the η-dependent model problem. The main technical issues consist of handling the overlapping of the spectral bands and clarifying the relations of the Floquet and spectral parameters especially as regards to integration by substitution.

We recall that the solution of the problem (1.1)–(1.3) can be written as

$$u(\cdot, t) = e^{\mathcal{T}t} g = \int_0^{\infty} e^{-\lambda t} dE_\lambda g = \int_\sigma e^{-\lambda t} dE_\lambda g, \tag{6.1}$$

where $(E_\lambda)_{\lambda\in[0,\infty)}$ is the resolution of the identity (see (3.14) of [45]) associated with the spectral measure $P(\Omega)$ of the operator $\mathcal{T}$ (Theorem 3.6. in [45], or Theorem VIII.6 of [40]) so that there holds $E_\lambda = P((-\infty,\lambda])$.

Given $k \in \mathbb{N}$, we decompose the interval $[-\pi,\pi]$ into finitely many subintervals $J_{k,q}$, $q = 1,\dots,q_k$, such that the mapping $\Lambda_k : \eta \mapsto \Lambda_k(\eta)$ is monotone, i.e. a bijection, on each of them and denote the inverse mappings $\eta_{k,q} : I_{k,q} \to J_{k,q}$, where $I_{k,q} = \Lambda_k(J_{k,q}) \subset \Upsilon_k$. This is possible because of Remark 3.3. Obviously, there holds the change of variables formula

$$\int\limits_{-\pi}^{\pi} f(\eta)d\eta = \sum_{q=1}^{q_k} \int\limits_{J_{k,q}} f(\eta)d\eta = \sum_{q=1}^{q_k} \int\limits_{I_{k,q}} f(\eta_{k,q}(\lambda))\eta'_{k,q}(\lambda)d\lambda, \tag{6.2}$$

where f is a scalar valued Lebesgue-integrable function or more generally a Banach-space valued Bochner-integrable function on $[-\pi,\pi]$. Note that here indeed k is arbitrary.

For every $\lambda \in \sigma$ we denote by $\mathbb{K}_\lambda \subset \mathbb{N}\times\mathbb{N}$ the (finite) set of all pairs (k,q) such that $\lambda \in I_{k,q} \subset \Upsilon_k$. The spectrum σ can be decomposed into a disjoint union of countably many subintervals such that the set-valued mapping $\lambda \mapsto \mathbb{K}_\lambda$ is constant on these subintervals. If $m \in \mathbb{N}$ is arbitrary, then Lemma 4.1 implies that there are at most m indices k such that $(k,q) \in \mathbb{K}_\lambda$ for some $\lambda \le C_\varpi m^{1/(dd^*)}$.

Formula (6.3) in the next definition looks complicated, but note that it simplifies a lot by applying the change of variables (6.2); see e.g. the second identity in (6.7).

Definition 6.1. For $\lambda \in \sigma$ and all pairs $(k,q) \in \mathbb{K}_\lambda$ we denote

$$F(x) := F(x;\lambda,k,q) = \begin{cases} \frac{1}{\sqrt{2\pi}} e^{i[x_1]\eta_{k,q}(\lambda)} G_k(\eta_{k,q}(\lambda)) V_k(x^{\mathrm{tr}};\eta_{k,q}(\lambda))\eta'_{k,q}(\lambda), & \lambda \in I_{k,q}, \\ 0, \quad \lambda \in \mathbb{R}_0^+ \setminus I_{k,q}, \end{cases} \tag{6.3}$$

where $x \in \Pi$, V_k is the eigenfunction (3.7) of the model problem and G_k is the inner product (5.9) for the function $g \in L^2(\Pi)$. For all $M > 0$ we also denote by $F_M = F_M(\cdot;\lambda,k,q)$ the restriction of F to the set $\Pi^M := \{x \in \Pi : |x| \le M\}$.

Note that usually F does not belong to $L^2(\Pi)$ or $L^1(\Pi)$, since its modulus is a periodic function. This fact complicates some of following calculations and the formulation of the results. Consequently, we need to formulate the following technical observation.

Lemma 6.2. *For all $M > 0$ the function*

$$\lambda \mapsto \sum_{(k,q)\in\mathbb{K}_\lambda} F_M(\cdot,\lambda,k,q) \tag{6.4}$$

is Bochner-integrable on $\sigma \cap I$ (as a function $\sigma \cap I \to L^2(\Pi^M)$), for every bounded interval I. Moreover, the limit

$$\lim_{M\to\infty} \int\limits_{\sigma\cap I} \sum_{(k,q)\in\mathbb{K}_\lambda} F_M(x;\lambda,k,q)\,d\lambda = \int\limits_{\sigma\cap I} \sum_{(k,q)\in\mathbb{K}_\lambda} F(x;\lambda,k,q)\,d\lambda, \tag{6.5}$$

converges in $L^2(\Pi)$.

Before proceeding with the proof, we remark that the sets $\mathbb{K}_\lambda$ are finite and depend piecewise constantly on $\lambda \in I$, hence, there are altogether only finitely many terms in the sums in (6.5). Thus, due to (5.10), (3.17) and the boundedness of the derivatives $\eta'_{k,q}$, both λ-integrals in (6.5) converge for every fixed $x \in \Pi$.

Proof. Let $M > 0$ and a bounded λ-interval I be given. Denoting by $\mathbb{K}(I)$ the finite set of all k such that the pair (k,q) appears in (6.4) for some $q = 1,\ldots,q_k$, we have by (3.10), (5.10), (6.3) and the definition of the notation x^{tr}

$$\begin{aligned}
&\int\limits_{\sigma\cap I} \Big\| \sum_{(k,q)\in\mathbb{K}_\lambda} F_M(x;\lambda,k,q) \Big\|_{\Pi^M} d\lambda, \\
&\quad\le \sum_{k\in\mathbb{K}(I)} \sum_{q=1}^{q_k} \int\limits_{I_{k,q}\cap I} \big\| e^{i[x_1]\eta_{k,q}(\lambda)} G_k(\eta_{k,q}(\lambda)) V_k(x^{\mathrm{tr}};\eta_{k,q}(\lambda))\eta'_{k,q}(\lambda) \big\|_{\Pi^M} d\lambda \\
&\quad\le CM \sum_{k\in\mathbb{K}(I)} \sum_{q=1}^{q_k} \int\limits_{I_{k,q}\cap I} \big\| V_k(x;\eta_{k,q}(\lambda)) \big\|_{\varpi} |\eta'_{k,q}(\lambda)| d\lambda \\
&\quad= CM \sum_{k\in\mathbb{K}(I)} \sum_{q=1}^{q_k} \int\limits_{J_{k,q}} \big\| V_k(x;\eta) \big\|_{\varpi} d\eta \le C'_I M < \infty.
\end{aligned} \tag{6.6}$$

This proves the Bochner-integrability.

Moreover, for a given $M > 0$ and for almost all $x \in \Pi^M$ (x fixed for a moment), the change of the integration variable (6.2) yields

$$\begin{aligned}
G_M(x) &:= \int\limits_{\sigma\cap I} \sum_{k\in\mathbb{K}(I)} \sum_{q=1}^{q_k} F_M(x,\lambda,k,q)\,d\lambda = \sum_{k\in\mathbb{K}(I)} \int\limits_{N_k} e^{i[x_1]\eta} G_k(\eta) V_k(x^{\mathrm{tr}};\eta) d\eta \\
&= \sum_{k\in\mathbb{K}(I)} \int\limits_{-\pi}^{\pi} e^{i[x_1]\eta} \chi_k(\eta) G_k(\eta) V_k(x^{\mathrm{tr}};\eta) d\eta = \sum_{k\in\mathbb{K}(I)} \mathsf{F}^{-1}\big(\chi_k(\eta) G_k(\eta) V_k(x;\eta)\big),
\end{aligned} \tag{6.7}$$

where N_k is a subset of the interval $[-\pi,\pi]$ (as Υ_k may not be completely contained in I) and χ_k is its characteristic function. If $x \in \Pi\setminus\Pi^M$, then the expression in (6.7), i.e., $G_M(x)$, is null, due the very definition of F_M.

Now, the function

$$H(x;\eta) := \sum_{k\in\mathbb{K}(I)} \chi_k(\eta) G_k(\eta) V_k(x;\eta)$$

belongs to $L^2(-\pi, \pi; L^2(\varpi))$, due to (3.10), (5.10), hence, $G := \mathsf{F}^{-1}H$ belongs to $L^2(\Pi)$, and by (6.7) we have $G_M(x) = G(x)$ for $x \in \Pi^M$. Since $G_M(x) = 0$ for x outside Π^M, we have $G_M \to G$ in $L^2(\Pi)$. Finally, the same calculation as in (6.7) shows that G coincides with the right-hand side of (6.5). □

In principle, the proof of the next theorem follows by changing the integration variables, but it is technically complicated by the problems mentioned in the beginning of this section.

Theorem 6.3. *If $g \in L^2(\Pi)$ is a function satisfying (1.4) and $t > 0$, then the limit*

$$\int_\sigma e^{-t\lambda} \sum_{(k,q)\in\mathbb{K}_\lambda} F(x, \lambda, k, q)\, d\lambda := \lim_{S\to\infty} \int_{\sigma\cap[0,S]} e^{-t\lambda} \sum_{(k,q)\in\mathbb{K}_\lambda} F(x, \lambda, k, q)\, d\lambda \tag{6.8}$$

converges in the space $L^2(\Pi)$ and it coincides with

$$e^{t\mathcal{T}} g(x) = \int_\sigma e^{-\lambda t} dE_\lambda g(x). \tag{6.9}$$

Proof. Fix $t > 0$, and then let $\varepsilon > 0$ be arbitrary. Fix $k_0 = k_0(t) \in \mathbb{N}$ such that

$$\sum_{k>k_0} e^{-t\gamma k^{2/d}} < \varepsilon^2 \tag{6.10}$$

where the constant γ is as in Lemma 4.1, and then, let λ_0 be any number such that

$$M_{k_0} \le \lambda_0 < M_{k_0+1}, \tag{6.11}$$

where M_{k_0} is the upper end of the spectral band Υ_{k_0}, see (3.20). Thus, for every $k \le k_0$, all bands Υ_k and intervals $I_{k,q} \subset \Upsilon_k$ with $k \le k_0$, $1 = 1, \dots, q_k$, are contained in $[0, \lambda_0]$.

Also, for $k > k_0$ it may still happen that $[0, \lambda_0] \cap \Upsilon_k \ne \emptyset$, which requires the next considerations. First, we denote by $K(\lambda_0)$ the set of those indices $k > k_0$ such that $\Upsilon_k \cap [0, \lambda_0] \ne \emptyset$. Moreover, for all $\lambda \le \lambda_0$, we denote

$$R_\lambda = \big\{(k, q) \in \mathbb{K}_\lambda \ : \ k > k_0\big\} \subset \mathbb{K}_\lambda, \tag{6.12}$$

where $\mathbb{K}_\lambda$ was defined before Definition 6.1; consequently, given $\lambda \le \lambda_0$, the set R_λ consists of all indices (k, q) such that $\lambda \in I_{k,q} \subset \Upsilon_k$ and $k > k_0$. Note that again, the set valued mapping $\lambda \mapsto R_\lambda$ is piecewise constant. Finally, for every $k \in K(\lambda_0)$ and $\lambda \in [0, \lambda_0]$ we also denote

$$Q_{k,\lambda} = \{q \ : \ (k, q) \in R_\lambda\} \subset \{1, \dots, q_k\}. \tag{6.13}$$

Note that also the set valued mapping $\lambda \to Q_{k,\lambda}$ is piecewise constant. The lower bound (4.1) implies that there exists a constant $C > 0$ (depending on ϖ only) such that for

$$k \ge C\lambda_0^{d/2} \tag{6.14}$$

we have $\Upsilon_k \cap [0, \lambda_0] = \emptyset$, hence, $k < C\lambda_0^{d/2}$ holds for every $k \in K(\lambda_0)$ with the same constant C as in (6.14).

By applying formula (6.2) and the definition of the sets $\mathbb{K}_\lambda$ and R_λ to all η-integrals, we get

$$\sum_{k=1}^{k_0} \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{i[x_1]\eta} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x^{\mathrm{tr}}; \eta) d\eta = \int_{\sigma\cap[0,\lambda_0]} \sum_{(k,q)\in\mathbb{K}_\lambda\setminus R_\lambda} e^{-t\lambda} F(x, \lambda, k, q)\, d\lambda. \tag{6.15}$$

Next, we derive an estimate for

$$\int_{\sigma\cap[0,\lambda_0]} \sum_{(k,q)\in R_\lambda} e^{-t\lambda} F(x, \lambda, k, q)\, d\lambda. \tag{6.16}$$

For a given $k \in K(\lambda_0)$, a change of the integration variable yields (cf. 6.8, 6.3)

$$\begin{aligned} \int_{\sigma\cap[0,\lambda_0]} \sum_{q\in Q_{k,\lambda}} e^{-t\lambda} F(x, \lambda, k, q)\, d\lambda &= \int_{N_k} e^{i[x_1]\eta} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x^{\mathrm{tr}}; \eta) d\eta \\ &= \sqrt{2\pi}\, \mathsf{F}^{-1}\big(\chi_{N_k} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x; \eta)\big), \end{aligned} \tag{6.17}$$

where N_k is a subset of the interval $[-\pi, \pi]$ (as Υ_k is not completely contained in $[0, \lambda_0]$, see above). Using (3.10), (5.10), (4.1) we can estimate

$$\begin{aligned} &\big\| \chi_{N_k} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x; \eta) \big\|^2_{L^2(-\pi,\pi;L^2(\varpi))} \\ &\quad = \int_{-\pi}^{\pi} \int_{\varpi} \big| \chi_{N_k} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x; \eta) \big|^2 dx d\eta \\ &\quad \le C e^{-\gamma k^{2/d} t} \int_{\varpi} |V_k(x; \eta)|^2 dx \le C e^{-\gamma k^{2/d} t}. \end{aligned} \tag{6.18}$$

Due to the isometric property of the Floquet transform we obtain from (6.17), (6.18) and (6.10)

$$\begin{aligned} &\Big\| \int_{\sigma\cap[0,\lambda_0]} \sum_{(k,q)\in R_\lambda} e^{-t\lambda} F(x, \lambda, k, q)\, d\lambda \Big\|_\Pi \\ &\quad \le \sum_{k\in K(\lambda_0)} \Big\| \int_{\sigma\cap[0,\lambda_0]} \sum_{q\in Q_{k,\lambda}} e^{-t\lambda} F(x, \lambda, k, q)\, d\lambda \Big\|_\Pi \\ &\quad = \sqrt{2\pi} \sum_{k\in K(\lambda_0)} \Big\| \chi_{N_k} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x; \eta) \Big\|_{L^2(-\pi,\pi;L^2(\varpi))} \\ &\quad \le \sum_{k\in K(\lambda_0)} C^{1/2} e^{-\frac{1}{2}\gamma k^{2/d} t} < C'\varepsilon, \end{aligned} \tag{6.19}$$

since $k > k_0$ for $k \in K(\lambda_0)$.

Taking into account (6.15), (6.19) yields

$$\Big\| \int\limits_{\sigma \cap [0,\lambda_0]} \sum_{(k,q)\in \mathbb{K}_\lambda} e^{-t\lambda} F(x,\lambda,k,q)\, d\lambda \\ - \sum_{k=1}^{k_0} \frac{1}{\sqrt{2\pi}} \int\limits_{-\pi}^{\pi} e^{i[x_1]\eta} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x^{\mathrm{tr}};\eta) d\eta \Big\|_\Pi < \varepsilon \tag{6.20}$$

for all large enough k_0 and λ_0 as in (6.11), hence, in view of the absolute convergence of the series (5.11) in $L^2(\Pi)$, the claims (6.8) and (6.9) are proved. □

Remark 6.4. In the proof of the next theorem we will need the trivial observation that the "scalar" versions of Lemma 6.2 and Theorem 6.3 also hold: given an arbitrary function $h \in L^2(\Pi)$, the function

$$\lambda \mapsto \sum_{(k,q)\in \mathbb{K}_\lambda} \big(F_M(\cdot,\lambda,k,q), h\big)_\Pi \tag{6.21}$$

is Lebesgue-integrable for every $M > 0$, and formulas (6.5), (6.8) holds, when the integrands are replaced on both sides with their $L^2(\Pi)$-inner products with h.

The following is a consequence of the previous theorem. Recall that $P(\Omega)$ denotes the spectral measure of the operator $\mathcal{T}$. Obviously, formula (6.22) determines the spectral measure in terms of the eigenfunctions of the model problem (5.1)–(5.4).

Theorem 6.5. *For every set $I = [a,b] \cap \sigma \subset \mathbb{R}_0^+$ with $0 \le a < b$ there holds the formula*

$$P(I)g(x) = \int\limits_I \sum_{(k,q)\in \mathbb{K}_\lambda} F(x,\lambda,k,q)\, d\lambda \tag{6.22}$$

where P is the spectral measure of the operator $\mathcal{T}$ in (1.5), $g \in L^2(\Pi)$, F is the expression (6.3) and the integral is defined by (6.5).

Proof. Functions g satisfying (1.4) form a dense subspace in $L^2(\Pi)$. Moreover, in addition to the orthogonal projection $P(I)$, also the sum on the right hand side of (6.22) defines a bounded operator $L^2(\Pi) \to L^2(\Pi)$,

$$g \mapsto \int\limits_I \sum_{(k,q)\in \mathbb{K}_\lambda} F(x,\lambda,k,q)\, d\lambda. \tag{6.23}$$

To see this, the right hand side of (6.22) or (6.23) equals, by using the substitution (6.2) as in (6.17), the expression

$$\sum_k \mathsf{F}^{-1}\big(\chi_k(\eta) G_k(\eta) V_k(x;\eta)\big) \tag{6.24}$$

where χ_k is the characteristic function of some subset of the interval $[-\pi, \pi]$ and the number of the terms is bounded by a constant not depending on g. Now, for all g in the unit ball B of $L^2(\Pi)$, the definition (5.9) implies that $|G_k(\eta)| \leq 1$, hence, the norm of $\chi_k G_k V_k$ in $L^2(-\pi, \pi; L^2(\varpi))$ is bounded by a constant independent of $g \in B$. Using the isometric property of F^{-1} shows that the $L^2(\Pi)$-norm of the right hand side of (6.24) is bounded by a constant independent of $g \in B$.

Hence, we may assume that (1.4) holds for g and thus the result of Theorem 6.3 can be used. Let $(e_n)_{n=1}^{\infty}$ be an orthonormal basis of the space $L^2(\Pi)$. Taking the inner product of (6.8), which is the same as (6.9), with any vector e_n yields the identity

$$\int_\sigma e^{-t\lambda}(dE_\lambda g, e_n)_\Pi = \int_\sigma e^{-t\lambda}\Big(\sum_{(k,q)\in\mathbb{K}_\lambda} F(x, \lambda, k, q), e_n\Big)_\Pi d\lambda \ \ \forall t > 0. \tag{6.25}$$

(Namely, on the left-hand side of (6.22), the definition of the spectral family or the resolution of the identity (E_λ) includes that the function $\lambda \mapsto (E_\lambda g, e_n)_\Pi$ is of bounded variation on every closed interval and thus the Stieltjes integral is well defined. On the right-hand side, to commute the integral and inner product, one needs to check all the steps of the definition of the integral and also use Remark 6.4.)

We interpret (6.25) as the equality of two standard scalar Laplace-Stieltjes transforms. Hence, the measures $(dE_\lambda g, e_n)_\Pi$ and $\big(\sum_{(k,q)\in\mathbb{K}_\lambda} F(x, \lambda, k, q), e_n\big)_\Pi d\lambda$ must be identical, and an integration with respect to λ over the set I yields

$$\big(P(I)g(x), e_n\big)_\Pi = \Big(\int_I \sum_{(k,q)\in\mathbb{K}_\lambda} F(x, \lambda, k, q)\, d\lambda, e_n\Big)_\Pi$$

for all $n \in \mathbb{N}$. This yields (6.22). □

7. Spectral projections of disjoint components

In this final section we consider the situation where the spectrum $\sigma = \sigma_{\text{ess}} \subset \mathbb{R}^+$ is not connected and thus contains a bounded disjoint component S. This may happen for example in the case when the adjacent periodic cells are connected with thin ligaments, see e.g. [36]. We will represent the spectral projection onto the subspace $H \subset L^2(\Pi)$, corresponding to the component S, by constructing an orthonormal basis of H consisting of Wannier functions and their translates. The results, of course, yield relevant information on the large time behavior of the solution of the heat equation (1.1)–(1.3). The emphasis here is in the simplicity of the presentation, and it should be mentioned that analogous results in other contexts are known to experts at least, see e.g. [25].

We assume that for some finite set $K \subset \mathbb{N}$ of indices,

$$S := \bigcup_{k\in K} \Upsilon_k \tag{7.1}$$

forms a disjoint, connected subset of the spectrum of $\mathcal{T}$, or, more generally, S of formula (7.1) is a finite union of such disjoint components of spectrum. We denote

$$\mathcal{H}_S = P(S)\mathcal{H}, \quad \text{where } P(S) = \int_S dE_\lambda \tag{7.2}$$

is the spectral projection corresponding to the component S.

Proposition 7.1. *The spectral projection $P(S)$ can be written as*

$$\begin{aligned} P(S)g(x) &= \frac{1}{\sqrt{2\pi}} \sum_{k\in K} \int_{-\pi}^{\pi} e^{i[x_1]\eta} G_k(\eta) V_k(x^{\mathrm{tr}}; \eta) d\eta \\ &= \sum_{k\in K} \mathsf{F}^{-1}\Big(\big(\mathsf{F}g(\cdot;\eta), V_k(\cdot;\eta)\big)_{\varpi} V_k(\cdot;\eta)\Big)(x), \end{aligned} \tag{7.3}$$

where $G_k(\eta)$ and V_k are as in (5.9) and (3.10), respectively. Consequently, if $g \in \mathcal{H}_S$, then the solution of the initial-boundary value problem (1.1)–(1.3) can be written as

$$e^{t\mathcal{T}} g = \int_0^\infty e^{-\lambda t} dE_\lambda g = \frac{1}{\sqrt{2\pi}} \sum_{k\in K} \int_{-\pi}^{\pi} e^{i[x_1]\eta} G_k(\eta) e^{-\Lambda_k(\eta)t} V_k(x_1 - [x_1], x'; \eta) d\eta. \tag{7.4}$$

Proof. From (6.22) we obtain

$$P(S)g(x) = \int_S \sum_{(k,q)\in\mathbb{K}_\lambda} F(x,\lambda,k,q)\, d\lambda, \tag{7.5}$$

and the same change of integration variables as in the proof of (6.15) shows that

$$\sum_{k\in K} \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{i[x_1]\eta} G_k(\eta) V_k(x^{\mathrm{tr}}; \eta) d\eta = \int_{\Upsilon_k} \sum_{(k,q)\in\mathbb{K}_\lambda} F(x,\lambda,k,q)\, d\lambda; \tag{7.6}$$

note that an analogue of the index set R_λ of formula (6.15) does not exist now, since we are assuming that Υ_k is separated from the other spectral bands Υ_k with $k \notin K$. □

Next we single out an orthonormal basis for the space $\mathcal{H}_S$. In the context of self-adjoint elliptic operators with periodic coefficients in $\mathbb{R}^d$, like the Schrödinger operators with periodic potentials, the functions (7.7) are called *Wannier functions*. See [25], Definition 3.1. We give an elementary proof for our case.

Theorem 7.2. *An orthonormal basis of the space $\mathcal{H}_S$ is formed by the functions*

$$\mathsf{F}^{-1} V_k(\cdot;\eta)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{i[x_1]\eta} V_k(x^{\mathrm{tr}}; \eta) d\eta \tag{7.7}$$

with $k \in K$ and all translates $\mathsf{F}^{-1} V_k \circ \tau_m$, $m \in \mathbb{Z}$.

Here, $f \circ \tau_m(x) = f(x_1 - m, x')$ for a function f of $x \in \Pi$.

Proof. Note that $\mathsf{F}^{-1} V_k(\cdot;\eta) \circ \tau_m = \mathsf{F}^{-1}(e^{-im\eta} V_k(\cdot;\eta))$. Denoting $h := \mathsf{F}^{-1} V_k(\cdot;\eta) \circ \tau_m$ we thus have for every $j \in K$, by (3.10),

$$\big(\mathsf{F}h(\cdot;\eta), V_j(\cdot,;\eta)\big)_{\varpi} = e^{-im\eta}\delta_{k,j} \tag{7.8}$$

so that $P(S)h = h$ follows from the representation of the spectral projection in (7.3). Moreover, if $k, j \in K$ and $m, n \in \mathbb{Z}$ are arbitrary, we have

$$\begin{aligned}\big(\mathsf{F}^{-1}V_k \circ \tau_m, \mathsf{F}^{-1}V_j \circ \tau_n\big)_\Pi &= \big(e^{im\eta}V_k, e^{in\eta}V_j\big)_{L^2(-\pi,\pi;L^2(\varpi))}\\ &= \int_{-\pi}^{\pi}\int_{\varpi} e^{i(m-n)\eta} V_k(x;\eta)\overline{V_j(x;\eta)}\,dx d\eta\\ &= \int_{-\pi}^{\pi} e^{i(m-n)\eta}\delta_{k,j} d\eta = \delta_{m,n}\delta_{k,j}.\end{aligned} \tag{7.9}$$

It remains to show that the functions span the subspace $\mathcal{H}_S$. Given $h \in L^2(\Pi)$, we first note that both functions $\mathsf{F}h(x;\eta)$ and $V_k(x;\eta)$ are 2π-periodic with respect to η, hence the inner product $G_k(\eta)$, defined as in (5.9) with h instead of g, is a continuous, periodic function on $[-\pi,\pi]$. We expand it as a Fourier series

$$G_k(\eta) = \sum_{n\in\mathbb{Z}} h_{k,n}e^{in\eta} \quad \text{with } (h_{k,n})_{n\in\mathbb{Z}} \in \ell^2(\mathbb{Z}) \tag{7.10}$$

and note that

$$\begin{aligned}P(S)h(x) &= \frac{1}{\sqrt{2\pi}}\sum_{k\in K}\int_{-\pi}^{\pi} e^{i[x_1]\eta}G_k(\eta)V_k(x^{\mathrm{tr}};\eta)d\eta\\ &= \frac{1}{\sqrt{2\pi}}\sum_{n\in\mathbb{Z}} h_{k,n}\sum_{k\in K}\int_{-\pi}^{\pi} e^{i[x_1]\eta}e^{in\eta}V_k(x^{\mathrm{tr}};\eta)d\eta\\ &= \sum_{n\in\mathbb{Z}} h_{k,n}\sum_{k\in K}\mathsf{F}^{-1}V_k \circ \tau_{-n}(x).\end{aligned} \tag{7.11}$$

The series converges in $L^2(\Pi)$, due to (7.10) and the observation in (7.9) that the functions $\mathsf{F}^{-1}V_k \circ \tau_{-n}$, $k \in K$, $n \in \mathbb{Z}$, form an orthonormal sequence. □

Let us finally consider the situation where the disjoint subset S of the spectrum in (7.1) consist of all bands Υ_k with $k = 1, 2, \ldots, N$ for some $N > 1$, i.e., the set K in (7.1) equals the sequence $(1, 2, \ldots, N)$. It is now plain from Theorem 7.2 that we have the decay rate

$$\|e^{t\mathcal{T}}g\|_\Pi \le Ce^{-m_{N+1}t}, \tag{7.12}$$

m_{N+1} as in (3.20), for all initial data g satisfying the orthogonality condition

$$\big(g, \mathsf{F}^{-1}V_k \circ \tau_m\big)_\Pi = 0 \quad \forall k \le N,\ m \in \mathbb{Z}. \tag{7.13}$$

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