Chapter 3

On the spectra of periodic differential operators

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The main mathematical tool for treating spectral problems for differential operators with periodic coefficients is the so-called Floquet–Bloch theory. It relates the spectrum of a selfadjoint operator realising a periodic spectral problem on the whole of $\mathbb{R}^n$ to a family of eigenvalue problems on the periodicity cell. Here, the eigenfunctions ("Bloch waves") are subject to semi-periodic boundary conditions depending on an additional parameter which varies over the so-called Brillouin zone. The result is the "band-gap" structure of the spectrum of the whole-space operator. Floquet–Bloch theory applies, in particular, to periodic Schrödinger equations and — what is most important within the scope of this book — to periodic Maxwell eigenvalue problems, i. e. to photonic crystals.

This theory is well-known to all experts, but it is not easy to find a self-contained exposition which moreover uses elementary arguments giving an easy access also for (doctoral) students. Since this book is mainly aiming at educating doctoral students, such a self-contained description is given here. On one hand, it is rather general because periodic differential operators of arbitrary even order are considered (which actually does not complicate the arguments), but on the other hand the coefficients are assumed to be "smooth", in order to satisfy our requirement of easy access. A more general exposition for non-smooth coefficients has been published in [2]. Important contributions to Floquet–Bloch theory have been made e. g. in [9, 10, 11].

Floquet–Bloch theory does not give an answer to the question if there are really gaps in the spectrum or if the bands actually overlap. An asymptotic answer (for sufficiently "high contrast" in the coefficients) has been given in [5]. In a more concrete case, existence of a gap has been proved by computer-assisted means in [8].

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3.1 The spectrum of selfadjoint operators

Here, we briefly summarise some basic results about the spectrum of selfadjoint linear operators

Definition. Let $(H, \langle\cdot,\cdot\rangle)$ denote a complex Hilbert space, $D(A) \subset H$ a dense subspace, and $A : D(A) \to H$ a linear operator.

a) The *adjoint* $A^* : D(A^*) \to H$ of A is defined by $D(A^*) := \{u \in H : \exists_{u^* \in H} \forall_{v \in D(A)} \langle u, Av\rangle = \langle u^*, v\rangle\}$ and $A^*u := u^*$ for $u \in D(A^*)$; note that, for $u \in D(A^*)$, u^* is unique.

b) A is *selfadjoint* iff $A = A^*$ (i. e. $D(A) = D(A^*)$, $Au = A^*u$ for $u \in D(A)$).

Definition. Let $A : D(A) \to H$ be a selfadjoint linear operator.

a) The *resolvent set* $\rho(A) \subset \mathbb{C}$ of A is defined as $\rho(A) := \{\lambda \in \mathbb{C} : A - \lambda I : D(A) \to H \text{ is bijective}\}$.

b) The *spectrum* of A is the set $\sigma(A) := \mathbb{C} \setminus \rho(A)$.

c) The *point spectrum* $\sigma_p(A)$ of A is the set of all eigenvalues of A.

d) The *continuous spectrum* $\sigma_c(A)$ of A is the set $\sigma_c(A) := \{\lambda \in \mathbb{C} : A - \lambda I \text{ is one-to-one but not onto}\}$.

Basic results.

i) For $\lambda \in \rho(A)$, $(A - \lambda I)^{-1}$ is bounded.

Proof. A is selfadjoint and hence closed, which implies that $(A - \lambda I)^{-1}$ is closed. Moreover, $(A - \lambda I)^{-1}$ is defined on H, whence its boundedness follows from the Closed Graph Theorem. □

ii) For all $\lambda \in \mathbb{C}, \mathrm{kernel}\,(\mathrm{A} - \lambda\mathrm{I}) = \mathrm{range}\,(\mathrm{A} - \lambda\mathrm{I})^\perp$.

Proof. If $u \in \mathrm{kernel}\,(\mathrm{A} - \lambda\mathrm{I}) \setminus \{0\}$, we have $\lambda \in \mathbb{R}$ since A is symmetric, and $\langle u, (A - \lambda I)v\rangle = \langle (A - \lambda I)u, v\rangle = 0$ for all $v \in D(A)$, i. e. $u \in \mathrm{range}\,(\mathrm{A} - \lambda\mathrm{I})^\perp$. If vice versa $u \in \mathrm{range}\,(\mathrm{A} - \lambda\mathrm{I})^\perp \setminus \{0\}$, we obtain $\langle u, Av\rangle = \langle \bar{\lambda}u, v\rangle$ for all $v \in D(A)$, whence the selfadjointness gives $u \in D(A)$, $Au = \bar{\lambda}u$, and $\lambda \in \mathbb{R}$ since A is symmetric, i. e. $u \in \mathrm{kernel}\,(\mathrm{A} - \lambda\mathrm{I})$. □

iii) For $\lambda \in \sigma_c(A), \mathrm{range}\,(\mathrm{A} - \lambda\mathrm{I})$ is dense in H (but not equal to H), and $(A - \lambda I)^{-1}$ is unbounded.

Proof. Since $A - \lambda I$ is one-to-one, $\mathrm{range}\,(\mathrm{A} - \lambda\mathrm{I})$ is dense in H by ii). If $(A - \lambda I)^{-1}$ were bounded, then (since $(A - \lambda I)^{-1}$ is closed) $\mathrm{range}\,(\mathrm{A} - \lambda\mathrm{I})$ would be closed, and hence equal to H, which contradicts the definition of $\sigma_c(A)$. □

iv) $\sigma(A) = \sigma_c(A) \,\dot{\cup}\, \sigma_p(A)$.

Proof. For each $\lambda \in \mathbb{C}$, $A - \lambda I$ is either bijective (i. e. $\lambda \in \rho(A)$), or one-to-one but not onto (i. e. $\lambda \in \sigma_c(A)$), or not one-to-one (i. e. $\lambda \in \sigma_p(A)$). This gives the result. □

v) $\sigma(A) \subset \mathbb{R}$

Proof. For $\lambda = \mu + \mathrm{i}\nu \in \mathbb{C}$, $\nu \neq 0$, we calculate $\|(A-\lambda I)u\|^2 = \|(A-\mu I)u\|^2 + \nu^2\|u\|^2 \geq \nu^2\|u\|^2$ for all $u \in D(A)$, which shows that $A - \lambda I$ is one-to-one, and $(A-\lambda I)^{-1}$ is bounded. So $\lambda \notin \sigma_p(A)$, and iii) shows that $\lambda \notin \sigma_c(A)$. Thus, $\lambda \in \rho(A)$ by iv). □

3.2 Periodic differential operators

Let $L(x, D) = \sum_{|\alpha| \leq m} c_\alpha(x) D^\alpha$ denote an m-th order linear differential operator on $\mathbb{R}^N$ with complex-valued and *periodic coefficients*, i. e. there exist linearly independent vectors $a_1, \ldots, a_N \in \mathbb{R}^N$ such that

$$c_\alpha(x + a_j) = c_\alpha(x) \qquad (x \in \mathbb{R}^N, |\alpha| \leq m, j = 1, \ldots, N)\,. \tag{3.1}$$

We assume that $L(\cdot, D)$ is uniformly strongly elliptic, i. e. m is even, and there exists $\delta > 0$ such that

$$(-1)^{\frac{m}{2}} \mathrm{Re}\left\{ \sum_{|\alpha|=m} c_\alpha(x) \xi^\alpha \right\} \geq \delta |\xi|^m \text{ for all } x, \xi \in \mathbb{R}^N.$$

(Note that the following assumption, together with (3.1), implies boundedness of the coefficients.) We suppose that

$$c_\alpha \in C^{|\alpha|}(\mathbb{R}^N) \text{ for } \alpha \neq (0, \ldots, 0),\ c_{(0,\ldots,0)} \in L^\infty(\mathbb{R}^N), \tag{3.2}$$

and that $L(\cdot, D)$ is *formally symmetric*, i. e. it coincides with its formal adjoint $L^*(\cdot, D)$ given by $L^*(\cdot, D)u = \sum_{|\alpha| \leq m} (-1)^{|\alpha|} D^\alpha(\bar{c}_\alpha u)$. This implies

$$\int\limits_{\mathbb{R}^N} [L(\cdot, D)u]\, \bar{v} dx = \int\limits_{\mathbb{R}^N} u \overline{L(\cdot, D) v} dx \tag{3.3}$$

for all $u, v \in C_0^\infty(\mathbb{R}^N)$, and hence, by denseness, for all $u, v \in H^m(\mathbb{R}^N)$. See also Chapter 1.2 for a description of the Lebesgue and Sobolev function spaces used here and in the following.

Furthermore, let $w \in L^\infty(\mathbb{R}^N)$ denote some real-valued weight function which is bounded from below by a positive constant, and which is also periodic in the sense (3.1). Thus, the complex Hilbert space $L^2(\mathbb{R}^N)$ can be endowed with the weighted scalar product

$$\langle u, v \rangle := \int\limits_{\mathbb{R}^N} w(x) u(x) \overline{v(x)}\, dx \qquad (u, v \in L^2(\mathbb{R}^N))$$

which is equivalent to the canonical (unweighted) one.

Now define an operator A in $L^2(\mathbb{R}^N)$ by

$$D(A) := H^m(\mathbb{R}^N), \ Au := \frac{1}{w} L(\cdot, D)u. \tag{3.4}$$

Lemma 3.2.1. *A is selfadjoint.*

Proof. By (3.3), (3.4), A is symmetric on $H^m(\mathbb{R}^N)$ with respect to $\langle \cdot, \cdot \rangle$, which implies that $H^m(\mathbb{R}^N) \subset D(A^*)$ and $Au = A^*u$ for $u \in H^m(\mathbb{R}^N)$. To prove the reverse inclusion $D(A^*) \subset H^m(\mathbb{R}^N)$, let $u \in D(A^*)$, i. e. $u \in L^2(\mathbb{R}^N)$ and there exists some $u^* \in L^2(\mathbb{R}^N)$ such that

$$\langle u, Av \rangle = \langle u^*, v \rangle \ \text{ for all } \ v \in H^m(\mathbb{R}^N). \tag{3.5}$$

Now let Ω denote some fundamental domain of periodicity (see also Section 3), and $\Omega_0 \supset \bar{\Omega}$ some additional bounded domain. $\mathbb{R}^N$ is the union (with measure zero overlap) of countably many translation copies $\bar{\Omega} + z_n$ ($n \in \mathbb{N}$) of $\bar{\Omega}$. (3.5) and (3.4) imply, for each $n \in \mathbb{N}$,

$$\int\limits_{\Omega_0 + z_n} u\overline{L(\cdot, D)v} dx = \int\limits_{\Omega_0 + z_n} w u^* \bar{v} dx \ \text{ for all } \ v \in C_0^\infty(\Omega_0 + z_n),$$

whence the transformation $x \to x - z_n$ and the periodicity of the coefficients give, for each $n \in \mathbb{N}$,

$$\int\limits_{\Omega_0} u(\cdot + z_n)\overline{L(\cdot, D)v} dx = \int\limits_{\Omega_0} w u^*(\cdot + z_n) \bar{v} dx \ \text{ for all } \ v \in C_0^\infty(\Omega_0).$$

Therefore, by [1, Thm. 6.3],

$$\begin{aligned} & u(\cdot + z_n)\big|_\Omega \in H^m(\Omega), \\ & \|u(\cdot + z_n)\|_{H^m(\Omega)} \le \gamma \left(\|u^*(\cdot + z_n)\|_{L^2(\Omega_0)} + \|u(\cdot + z_n)\|_{L^2(\Omega_0)} \right), \end{aligned} \tag{3.6}$$

where γ depends only on $L(\cdot, D), \Omega, \Omega_0$, and w. Squaring this inequality and transforming $x \to x + z_n$ in the integrals in the norms we obtain

$$\|u\|^2_{H^m(\Omega + z_n)} \le 2\gamma^2 \left(\|u^*\|^2_{L^2(\Omega_0 + z_n)} + \|u\|^2_{L^2(\Omega_0 + z_n)} \right).$$

Here, the right-hand side is summable over $n \in \mathbb{N}$ since Ω_0 intersects only with finitely many of the (disjoint) translation copies of Ω, and $u, u^* \in L^2(\mathbb{R}^N)$. Hence also the left-hand side is summable, implying $u \in H^m(\mathbb{R}^N)$. $\square$

Remarks.

a) We can alternatively assume that $L(\cdot, D)$ is given in divergence form $\sum_{|\alpha|,|\beta|\le m/2}(-1)^{|\alpha|}D^\alpha(c_{\alpha\beta}D^\beta)$. Then the formal symmetry simply reads $c_{\alpha\beta} = \overline{c_{\beta\alpha}}$. Instead of (3.2), we now require

$$c_{\alpha\beta} \in C^{\frac{m}{2}}(\mathbb{R}^N) \tag{3.7}$$

which is weaker than (3.2) for the "higher order" coefficients, but stronger for the "lower order" ones. Under these assumptions (together with uniform strong ellipticity), we can use [6, Thm. 16.1] (instead of [1]) to obtain the crucial statement (3.6) in the proof of Lemma 3.2.1.

b) Both alternative smoothness assumptions (3.2) and (3.7) may be regarded as unpleasant in view of some applications. In [2], a more general (but technically more involved) theory is presented where $L(\cdot, D)$ is given in divergence form, with the coefficients $c_{\alpha\beta}$ assumed to be merely in $L^\infty(\mathbb{R}^N)$ (and periodic). Here, the underlying Hilbert space is chosen to be the dual space $H^{-m/2}(\mathbb{R}^N)$.

c) For a general description of the construction of selfadjoint operators from formally selfadjoint differential expressions, see e. g. the books [3, 7, 11].

Our aim is now to prove a "band-gap" structure of the spectrum of A, i. e. to prove that the spectrum of A is a union of compact intervals. The proof will furthermore give access to computation of these spectral bands via eigenvalue problems on bounded domains.

3.3 Fundamental domain of periodicity and the Brillouin zone

Let Ω be a fundamental domain of periodicity associated with (3.1). For example, Ω can be chosen to be the $N-$dimensional parallelogram which has the origin in $\mathbb{R}^N$ as one corner, and the vectors a_j forming the sides which meet at that corner. But there is a lot of freedom in choosing Ω. (If e. g. $N = 2$, $a_1 = (1, 0)^T$, $a_2 = (0, 1)^T$, then $\Omega = (0, 1)^2$ can be chosen, but as well the parallelogram spanned by $\widetilde{a_1} = (1, 0)^T$, $\widetilde{a_2} = (1, 1)^T$.)

Next, let $b_1, \ldots, b_N \in \mathbb{R}^N$ denote the columns of $2\pi(M^T)^{-1}$, with M denoting the matrix with columns $a_1, \ldots, a_N$. Hence

$$b_l \cdot a_j = 2\pi\delta_{lj} \qquad (l, j = 1, \ldots, N)\,. \tag{3.8}$$

$b_1, \ldots, b_N$ generate a new periodicity lattice in $\mathbb{R}^N$, the so-called *reciprocal lattice*. As before, we can choose a fundamental domain of periodicity. A particular choice is the set of all points in $\mathbb{R}^N$ which are closer to 0 than to any other point in the reciprocal lattice. This set is called *Brillouin zone* B.

3.4 Bloch waves, Floquet transformation

For fixed $k \in \overline{B}$, we consider the eigenvalue problem

$$L(\cdot, D)\psi = \lambda w \psi \quad \text{on } \Omega\,, \tag{3.9}$$

$$\psi(x + a_j) = e^{\mathrm{i}k\cdot a_j}\psi(x) \qquad (j = 1, \dots, N)\,. \tag{3.10}$$

In writing the boundary condition in the form (3.10), we understand ψ extended to the whole of $\mathbb{R}^N$. In fact, (3.10) forms boundary conditions on $\partial\Omega$, so-called *semi-periodic* boundary conditions.

Since $L(\cdot, D)$ is formally symmetric and the coefficients of L, as well as the weight function w, are periodic with domain of periodicity Ω, we conclude that (3.9), (3.10) is a *symmetric* eigenvalue problem in $L^2(\Omega; w)$. Since Ω is bounded, compactness arguments can be used to prove that (3.9), (3.10) has a $\langle\cdot,\cdot\rangle$-orthonormal and complete system $(\psi_s(\cdot, k))_{s\in\mathbb{N}}$ of eigenfunctions in $H^m_{loc}(\mathbb{R}^N)$, with corresponding eigenvalues satisfying

$$\lambda_1(k) \le \lambda_2(k) \le \cdots \le \lambda_s(k) \to \infty \text{ as } s \to \infty\,. \tag{3.11}$$

The eigenfunctions $\psi_s(\cdot, k)$ are called *Bloch waves.* They can be chosen such that they depend on k in a measurable way (see [11, XIII.16, Theorem XIII.98]).

Now define

$$\phi_s(x, k) := e^{-\mathrm{i}k\cdot x}\psi_s(x, k)\,. \tag{3.12}$$

Then,

$$D^\alpha\psi_s(\cdot, k) = e^{\mathrm{i}k\cdot x}(D + \mathrm{i}k)^\alpha\phi_s(\cdot, k)$$

and thus

$$L(\cdot, D)\psi_s(\cdot, k) = e^{\mathrm{i}k\cdot x}L(\cdot, D + \mathrm{i}k)\phi_s(\cdot, k)\,. \tag{3.13}$$

Furthermore, using (3.10) and (3.12),

$$\phi_s(x + a_j, k) = e^{-\mathrm{i}k\cdot(x+a_j)}\psi_s(x + a_j, k) = \phi_s(x, k)\,,$$

which together with (3.13) shows that $(\phi_s(\cdot, k))_{s\in\mathbb{N}}$ is an orthonormal and complete system of eigenfunctions of the *periodic* eigenvalue problem

$$L(\cdot, D + \mathrm{i}k)\phi = \lambda w \phi \quad \text{on } \Omega\,, \tag{3.14}$$

$$\phi(x + a_j) = \phi(x) \qquad (j = 1, \dots, N)\,,$$

with the same eigenvalue sequence $(\lambda_s(k))_{s\in\mathbb{N}}$ as before. We shall see that the spectrum of the operator A can be constructed from the eigenvalue sequences $(\lambda_s(k))_{s\in\mathbb{N}}$ by varying k over the Brillouin zone B.

An important step towards this aim is the *Floquet transformation*

$$(Uf)(x,k) := \frac{1}{\sqrt{|B|}} \sum_{n\in\mathbb{Z}^N} f(x-Mn)e^{\mathrm{i}k^T Mn} \qquad (x\in\Omega, k\in B)\,, \tag{3.15}$$

recalling that M denotes the matrix with columns $a_1,\dots,a_N$.

Lemma 3.4.1. *$U : L^2(\mathbb{R}^N) \to L^2(\Omega\times B)$ is an isometric isomorphism, with inverse*

$$(U^{-1}g)(x-Mn) = \frac{1}{\sqrt{|B|}} \int_B g(x,k)e^{-\mathrm{i}k^T Mn}\,dk \qquad (x\in\Omega, n\in\mathbb{Z}^N)\,. \tag{3.16}$$

If $g(\cdot,k)$ is extended to the whole of $\mathbb{R}^N$ by the semi-periodicity condition (3.10), *we have*

$$U^{-1}g = \frac{1}{\sqrt{|B|}} \int_B g(\cdot,k)\,dk. \tag{3.17}$$

Proof. For $f\in L^2(\mathbb{R}^N)$,

$$\int_{\mathbb{R}^N} w|f(x)|^2\,dx = \sum_{n\in\mathbb{Z}^N} \int_\Omega w|f(x-Mn)|^2\,dx\,. \tag{3.18}$$

Here, we can exchange summation and integration by Beppo Levi's Theorem. Therefore,

$$\sum_{n\in\mathbb{Z}^N} |f(x-Mn)|^2 < \infty \quad \text{for a.e. } x\in\Omega\,.$$

Thus, $(Uf)(x,k)$ is well defined by (3.15) (as a Fourier series with variable $M^T k$) for a. e. $x\in\Omega$, and Parseval's equality gives, for these x,

$$\int_B |(Uf)(x,k)|^2\,dk = \sum_{n\in\mathbb{Z}^N} |f(x-Mn)|^2\,.$$

By (3.18), this expression is in $L^2(\Omega)$, and

$$\|Uf\|_{L^2(\Omega\times B)} = \|f\|_{L^2(\mathbb{R}^N)}\,.$$

We are left to show that U is onto, and that U^{-1} is given by (3.16) or (3.17). Let $g\in L^2(\Omega\times B)$, and define

$$f(x-Mn) := \frac{1}{\sqrt{|B|}} \int_B g(x,k)e^{-\mathrm{i}k^T Mn}\,dk \qquad (x\in\Omega, n\in\mathbb{Z}^N)\,. \tag{3.19}$$

For fixed $x \in \Omega$, Plancherel's Theorem gives

$$\sum_{n\in\mathbb{Z}^N} |f(x-Mn)|^2 = \int_B |g(x,k)|^2\,dk\,,$$

whence, by integration over Ω,

$$\begin{aligned}\int_{\Omega\times B} w|g(x,k)|^2\,dxdk &= \int_\Omega \sum_{n\in\mathbb{Z}^N} w|f(x-Mn)|^2\,dx\\ &= \sum_{n\in\mathbb{Z}^N}\int_\Omega w|f(x-Mn)|^2\,dx = \int_{\mathbb{R}^N} w|f(x)|^2\,dx\,,\end{aligned}$$

i. e. $f \in L^2(\mathbb{R}^N)$. Now (3.15) gives, for a. e. $x \in \Omega$,

$$f(x-Mn) = \frac{1}{\sqrt{|B|}}\int_B (Uf)(x,k)e^{-\mathrm{i}k^TMn}\,dk \qquad (n\in\mathbb{Z}^N)\,,$$

whence (3.19) implies $Uf = g$ and (3.16). Now (3.17) follows from (3.16) using $g(x+Mn,k) = e^{\mathrm{i}k^TMn}g(x,k)$. □

3.5 Completeness of the Bloch waves

Using the Floquet transformation U, we are now able to prove a completeness property of the Bloch waves $\psi_s(\cdot,k)$ in $L^2(\mathbb{R}^N)$ when we vary k over the Brillouin zone B.

Theorem 3.5.1. *For each $f \in L^2(\mathbb{R}^N)$ and $l \in \mathbb{N}$, define*

$$f_l(x) := \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \langle (Uf)(\cdot,k),\psi_s(\cdot,k)\rangle_{L^2(\Omega;w)}\,\psi_s(x,k)\,dk \quad (x\in\mathbb{R}^N)\,. \quad (3.20)$$

Then, $f_l \to f$ in $L^2(\mathbb{R}^N)$ as $l \to \infty$.

Proof. Since $Uf \in L^2(\Omega\times B)$, we have $(Uf)(\cdot,k) \in L^2(\Omega)$ for a. e. $k \in B$ by Fubini's Theorem. Since $(\psi_s(\cdot,k))_{s\in\mathbb{N}}$ is orthonormal and complete in $L^2(\Omega;w)$ for each $k \in B$, we obtain

$$\lim_{l\to\infty}\|(Uf)(\cdot,k) - g_l(\cdot,k)\|_{L^2(\Omega;w)} = 0 \quad \text{for a. e. } k\in B$$

where

$$g_l(x,k) := \sum_{s=1}^{l}\langle (Uf)(\cdot,k),\psi_s(\cdot,k)\rangle_{L^2(\Omega;w)}\,\psi_s(x,k)\,. \qquad (3.21)$$

Thus, for $\chi_l(k) := \|(Uf)(\cdot,k) - g_l(\cdot,k)\|^2_{L^2(\Omega;w)}$, we get

$$\chi_l(k) \to 0 \text{ as } l \to \infty \quad \text{for a. e. } k \in B\,,$$

and moreover, by Bessel's inequality,

$$\chi_l(k) \leq \|(Uf)(\cdot,k)\|^2_{L^2(\Omega;w)} \quad \text{for all } l \in \mathbb{N} \text{ and a. e. } k \in B\,,$$

and $\|(Uf)(\cdot,k)\|^2_{L^2(\Omega;w)}$ is in $L^1(B)$ as a function of k, by Lemma 3.4.1. Altogether, Lebesgue's Dominated Convergence Theorem implies

$$\int\limits_B \chi_l(k)\,dk \to 0 \text{ as } l \to \infty\,,$$

i. e.,

$$\|Uf - g_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty\,. \tag{3.22}$$

Using (3.20), (3.21), and (3.17), we find that $f_l = U^{-1}g_l$, whence (3.22) gives

$$\|U(f - f_l)\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty\,,$$

and the assertion follows since $U : L^2(\mathbb{R}^N) \to L^2(\Omega \times B)$ is isometric by Lemma 3.4.1. □

3.6 The spectrum of A

In this section, we will prove the main result stating that

$$\sigma(A) = \bigcup_{s\in\mathbb{N}} I_s\,, \tag{3.23}$$

where

$$I_s := \{\lambda_s(k) : k \in \overline{B}\} \qquad (s \in \mathbb{N})\,. \tag{3.24}$$

For each $s \in \mathbb{N}$, λ_s is a continuous function of $k \in \overline{B}$, which follows by standard arguments from the fact that the coefficients in the eigenvalue problem (3.14) depend continuously on k. Thus, since $\overline{B}$ is compact and connected,

$$I_s \text{ is a compact real interval, for each } s \in \mathbb{N}\,. \tag{3.25}$$

Moreover, Poincaré's min-max principle for eigenvalues implies that

$$\mu_s \leq \lambda_s(k) \quad \text{for all } s \in \mathbb{N},\ k \in \overline{B}\,,$$

with $(\mu_s)_{s\in\mathbb{N}}$ denoting the sequence of eigenvalues of problem (3.9) with *Neumann* ("free") boundary conditions. Since $\mu_s \to \infty$ as $s \to \infty$, we obtain

$$\min I_s \to \infty \text{ as } s \to \infty\,, \tag{3.26}$$

which together with (3.25) implies that

$$\bigcup_{s\in\mathbb{N}} I_s \text{ is closed}\,. \tag{3.27}$$

The first part of the statement (3.23) is

Theorem 3.6.1. $\sigma(A) \supset \bigcup_{s\in\mathbb{N}} I_s$.

Proof. Let $\lambda \in \bigcup_{s\in\mathbb{N}} I_s$, i. e. $\lambda = \lambda_s(k)$ for some $s \in \mathbb{N}$ and some $k \in \overline{B}$, and

$$L(\cdot, D)\psi_s(\cdot, k) = \lambda w \psi_s(\cdot, k)\,. \tag{3.28}$$

We regard $\psi_s(\cdot, k)$ as extended to the whole of $\mathbb{R}^N$ by the boundary condition (3.10), whence, due to the periodicity of the coefficients of $L(\cdot, D)$, (3.28) holds for all $x \in \mathbb{R}^N$.

We choose a function $\eta \in C_0^\infty(\mathbb{R}^N)$ such that

$$\eta(x) = 1 \quad \text{for } |x| \le 1, \quad \eta(x) = 0 \quad \text{for } |x| \ge 2\,,$$

and define, for each $l \in \mathbb{N}$,

$$u_l(x) := \eta\left(\frac{|x|}{l}\right)\psi_s(x, k)\,.$$

Then,

$$\begin{aligned} (L(\cdot, D) - \lambda w)u_l &= \sum_{|\alpha|\le m} c_\alpha D^\alpha \left[\eta\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot, k)\right] - \lambda w \eta\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot, k) \qquad (3.29) \\ &= \eta\left(\frac{|\cdot|}{l}\right)(L(\cdot, D) - \lambda w)\psi_s(\cdot, k) + R\,, \end{aligned}$$

where R is a sum of products of bounded functions, derivatives (of order ≥ 1) of $\eta\left(\frac{|\cdot|}{l}\right)$, and derivatives (of order $\le m-1$) of $\psi_s(\cdot, k)$. Thus (note that $\psi_s(\cdot, k) \in H^m_{\mathrm{loc}}(\mathbb{R}^N)$),

$$\|R\|_{L^2(\mathbb{R}^N)} \le \frac{c}{l}\|\psi_s(\cdot, k)\|_{H^{m-1}(K_{2l})}\,, \tag{3.30}$$

with K_{2l} denoting the ball in $\mathbb{R}^N$ with radius $2l$, centered at 0. Moreover, the semi-periodic structure of $\psi_s(\cdot, k)$ implies

$$\|\psi_s(\cdot, k)\|_{H^{m-1}(K_{2l})} \le c\sqrt{\mathrm{vol}(\mathrm{K}_{2l})}\,.$$

Together with (3.28), (3.29), (3.30), this gives

$$\|(L(\cdot, D) - \lambda w)u_l\|_{L^2(\mathbb{R}^N)} \leq \frac{c}{l}\sqrt{\mathrm{vol}(\mathrm{K}_{2l})}\,.$$

Furthermore, again by the semiperiodic structure of $\psi_s(\cdot, k)$,

$$\|u_l\|_{L^2(\mathbb{R}^N)} \geq c\|\psi_s(\cdot, k)\|_{L^2(K_l)} \geq c\sqrt{\mathrm{vol}(\mathrm{K}_l)}$$

with $c > 0$. Since $\mathrm{vol}(\mathrm{K}_{2l})/\mathrm{vol}(\mathrm{K}_l)$ is bounded, we obtain

$$\frac{1}{\|u_l\|_{L^2(\mathbb{R}^N)}}\|(L(\cdot, D) - \lambda w)u_l\|_{L^2(\mathbb{R}^N)} \leq \frac{c}{l}\,.$$

Because moreover $u_l \in H^m(\mathbb{R}^N) = D(A)$, this results in

$$\frac{1}{\|u_l\|_{L^2(\mathbb{R}^N)}}\|(A - \lambda I)u_l\|_{L^2(\mathbb{R}^N)} \to 0 \text{ as } l \to \infty\,.$$

Thus, either λ is an eigenvalue of A, or $(A - \lambda I)^{-1}$ exists but is unbounded. In both cases, $\lambda \in \sigma(A)$ by the result i) in Section 1. □

Now we turn to the reverse statement

Theorem 3.6.2. $\sigma(A) \subset \bigcup_{s\in\mathbb{N}} I_s$

Proof. Let $\lambda \in \mathbb{R} \setminus \bigcup_{s\in\mathbb{N}} I_s$. We have to prove that $\lambda \in \rho(A)$, i. e., that, for each $f \in L^2(\mathbb{R}^N)$, some $u \in D(A)$ exists satisfying $(A - \lambda I)u = f$. (Then, $A - \lambda I$ is onto, and hence also one-to-one by the basic result ii) in Section 1.) For given $f \in L^2(\mathbb{R}^N)$, we define, for $l \in \mathbb{N}$,

$$f_l(x) := \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \langle (Uf)(\cdot, k),\, \psi_s(\cdot, k)\rangle_{L^2(\Omega;w)}\psi_s(x, k)\, dk$$

and

$$u_l(x) := \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \frac{1}{\lambda_s(k) - \lambda}\langle (Uf)(\cdot, k),\, \psi_s(\cdot, k)\rangle_{L^2(\Omega;w)}\psi_s(x, k)\, dk\,. \quad (3.31)$$

Here, we note that, due to (3.27), some $\delta > 0$ exists such that

$$|\lambda_s(k) - \lambda| \geq \delta \quad \text{for all } s \in \mathbb{N},\, k \in B\,. \quad (3.32)$$

In particular, the boundary value problem

$$\begin{aligned}(L(\cdot, D) - \lambda w)v(\cdot, k) &= w(Uf)(\cdot, k) \text{ in } \Omega\,, \\ v(x + a_j) &= e^{\mathrm{i}k\cdot a_j}v(x) \qquad (j = 1, \ldots, N)\end{aligned} \quad (3.33)$$

has a unique solution for every $k \in B$. Bloch wave expansion gives

$$\begin{aligned}\|(Uf)(\cdot,k)\|^2_{L^2(\Omega;w)} &= \sum_{s=1}^{\infty} |\langle (Uf)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)}|^2 \\ &= \sum_{s=1}^{\infty} |\langle (w^{-1}L(\cdot,D)-\lambda)v(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)}|^2 \,.\end{aligned}$$

Since both $v(\cdot,k)$ and $\psi_s(\cdot,k)$ satisfy semi-periodic boundary conditions, $w^{-1}L(\cdot,D)-\lambda$ can be moved to $\psi_s(\cdot,k)$ in the inner product, and hence (3.9) and (3.32) give

$$\begin{aligned}\|(Uf)(\cdot,k)\|^2_{L^2(\Omega;w)} &= \sum_{s=1}^{\infty} |\lambda_s(k)-\lambda|^2 |\langle v(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)}|^2 \\ &\geq \delta^2 \|v(\cdot,k)\|^2_{L^2(\Omega;w)} \,.\end{aligned}$$

By Lemma 3.4.1, this implies $v \in L^2(\Omega \times B)$, and we can define $u := U^{-1}v \in L^2(\mathbb{R}^N)$. Thus, (3.33) gives

$$\begin{aligned}\langle (Uf)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)} &= \langle (w^{-1}L(\cdot,D)-\lambda)(Uu)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)} \\ &= \langle (Uu)(\cdot,k),\, (w^{-1}L(\cdot,D)-\lambda)\psi_s(\cdot,k)\rangle_{L^2(\Omega;w)} \\ &= (\lambda_s(k)-\lambda)\langle Uu(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)} \,,\end{aligned}$$

whence (3.31) implies

$$u_l(x) = \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uu)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)} \psi_s(x,k)\, dk \,, \tag{3.34}$$

and Theorem 3.5.1 gives

$$u_l \to u, \quad f_l \to f \quad \text{in } L^2(\mathbb{R}^N) \,. \tag{3.35}$$

We will now prove that (in the distributional sense)

$$(w^{-1}L(\cdot,D)-\lambda)u_l = f_l \quad \text{for all } l \in \mathbb{N} \,, \tag{3.36}$$

which implies (compare (3.37) below) that $\langle u_l, (A-\lambda I)v\rangle = \langle f_l, v\rangle$ for all $v \in H^m(\mathbb{R}^N) = D(A)$, whence Lemma 3.2.1 implies $u_l \in D(A)$, and

$$(A-\lambda I)u_l = f_l \quad \text{for all } l \in \mathbb{N} \,.$$

Since A is closed, (3.35) now implies

$$u \in D(A), \text{ and } (A-\lambda I)u = f \,,$$

which is the desired result.

We are left to prove (3.36), i. e. that

$$\langle u_l,\, (w^{-1}L(\cdot,D)-\lambda)\varphi\rangle_{L^2(\mathbb{R}^N)} = \langle f_l, \varphi\rangle_{L^2(\mathbb{R}^N)} \quad \text{for all } \varphi \in C_0^\infty(\mathbb{R}^N). \tag{3.37}$$

So let $\varphi \in C_0^\infty(\mathbb{R}^N)$ be fixed, and let $K \subset \mathbb{R}^N$ denote a ball containing $\operatorname{supp}(\varphi)$ in its interior. Both the functions

$$\begin{aligned} r_s(x,k) &:= w(x)\frac{1}{\lambda_s(k)-\lambda}\langle (Uf)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)} \\ &\qquad \psi_s(x,k)\overline{(w^{-1}L(x,D)-\lambda)\varphi(x)}\,, \\ t_s(x,k) &:= w(x)\langle (Uf)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)}\psi_s(x,k)\overline{\varphi(x)} \end{aligned}$$

are easily seen to be in $L^2(K\times B)$ by Fubini's Theorem, since (3.32), and the fact that $(w^{-1}L(\cdot,D)-\lambda)\varphi \in L^\infty(K)$ and $\varphi \in L^\infty(K)$, imply that both

$$\int_K |r_s(x,k)|^2\,dx$$

and

$$\int_K |t_s(x,k)|^2\,dx$$

are bounded by

$$C\|(Uf)(\cdot,k)\|^2_{L^2(\Omega;w)}\|\psi_s(\cdot,k)\|^2_{L^2(K)}\,;$$

the latter factor is bounded as a function of k because K is covered by a finite number of copies of Ω, and the former is in $L^1(B)$ by Lemma 3.4.1.

Since $K\times B$ is bounded, r and t are also in $L^1(K\times B)$. Therefore, Fubini's Theorem implies that the order of integration with respect to x and k may be exchanged for r and t. Thus, by (3.31),

$$\begin{aligned} &\int\limits_K w(x)u_l(x)\overline{(w^{-1}L(x,D)-\lambda)\varphi(x)}\,dx \\ &\qquad = \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int\limits_K\left(\int\limits_B r_s(x,k)\,dk\right)dx \\ &\qquad = \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int\limits_B \frac{1}{\lambda_s(k)-\lambda}\langle (Uf)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)} \\ &\qquad\qquad\qquad \langle \psi_s(\cdot,k),\, (w^{-1}L(\cdot,D)-\lambda)\varphi\rangle_{L^2(K;w)}\,dk\,. \end{aligned}$$

Since φ has compact support in the interior of K, $w^{-1}L(\cdot,D)-\lambda$ may be moved to $\psi_s(\cdot, k)$, and hence (3.9) gives

$$\begin{aligned}
&\int_K w(x)u_l(x)\overline{(w^{-1}L(x,D)-\lambda)\varphi(x)}\,dx \\
&\quad = \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \langle (Uf)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)}\langle \psi_s(\cdot,k),\varphi\rangle_{L^2(K;w)}\,dk \\
&\quad = \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \left(\int_K t_s(x,k)\,dx\right)dk \\
&\quad = \int_K w(x)\left[\frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \langle (Uf)(\cdot,k),\, \psi_s(\cdot,k)\rangle_{L^2(\Omega;w)}\psi_s(x,k)\,dk\right]\overline{\varphi(x)}\,dx \\
&\quad = \int_K w(x)f_l(x)\overline{\varphi(x)}\,dx,
\end{aligned}$$

i. e. (3.37). □

Theorems 3.6.1 and 3.6.2 give the result (3.23). It is however difficult to decide, whether there are really *gaps* in the union (3.23). Moreover, it is not easy to make statements about the nature of the spectrum $\sigma(A)$, for example to decide if $\sigma(A) = \sigma_c(A)$ (i. e. no eigenvalues occur). The only easy result is

Theorem 3.6.3. *$\sigma(A)$ contains no eigenvalues of finite multiplicity.*

Proof. (See [4]) Let λ be an eigenvalue of A and suppose that $E := \mathrm{kernel}(A - \lambda I)$ is finite dimensional. The periodicity of the coefficients of $L(\cdot, D)$ shows that $f \in E$ implies $f(\cdot\ + a_1) \in E$. Thus, the mapping

$$V : \left\{ \begin{array}{l} E \to E \\ f \mapsto f(\cdot\ + a_1) \end{array} \right\}$$

is well defined, and moreover

$$\langle Vf, Vg\rangle_{L^2(\mathbb{R}^N)} = \langle f, g\rangle_{L^2(\mathbb{R}^N)} \text{ for } f, g \in E,$$

i. e. V is unitary. The assumption $\dim E < \infty$ implies that V has at least one eigenvalue $\kappa \in \mathbb{C}$, and $|\kappa| = 1$ since V is unitary. An eigenfunction $f \in E \setminus \{0\}$ of V, associated with κ, satisfies $f(\cdot + a_1) \equiv \kappa f$, and thus $|f(x + a_1)| = |f(x)|$ for all $x \in \mathbb{R}^N$, which contradicts $f \in L^2(\mathbb{R}^N)$. □

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