1 On the spectra of Schrödinger operator with periodic delta potential

1.1 Periodic differential operator

1.2 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 $L^2(\Omega)$ when we vary k over the Brillouin zone B.

Theorem 1.1. *For each $f \in L^2(\mathbb{R})$ and $l \in \mathbb{N}$, define*

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, K) dk \quad (x \in \mathbb{R}). \tag{1.1}$$

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

Beweis. Sine $Uf \in L^2(\Omega \times B)$, 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 $L^2(\Omega)$ for each $k \in B$, we obtain

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

where

$$g_l(x, k) := \sum_{s=1}^{l} \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k). \tag{1.2}$$

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

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

and moreover, by Bessel's inequality,

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

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

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

i.e.,

$$\|Uf - g_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty \tag{1.3}$$

Using (1.1), (1.2) and (**??**), we find that $f_l = U^{-1}g_l$, whence (1.3) gives

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

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

1.3 The spectrum of A

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

$$\sigma(A) = \bigcup_{s\in\mathbb{N}} I_s \tag{1.4}$$

where

$$I_s \coloneqq \{\lambda_s(k) : k \in \overline{B}\} \quad (s \in \mathbb{N})$$

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 (**??**), (**??**) depend continuously on k. Thus, since B is compact and connected,

$$I_s \text{ is a compact real interval, for each } s \in \mathbb{N}. \tag{1.5}$$

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

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

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

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

which together with (1.5) implies that

$$\bigcup_{s\in\mathbb{N}} I_s \text{ is close.}$$

The first part of the statement (1.4) is

Theorem 1.2. $\sigma(A) \supset \bigcup_{s\in\mathbb{N}} I_s$.

Beweis. 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

$$A\psi_s(\cdot,k) = \lambda\psi_s(\cdot,k) \tag{1.6}$$

We regard $\psi_s(\cdot,k)$ as extended to the whole of $\mathbb{R}$ by the boundary condition (**??**), whence, due to the periodicity of A, (1.6) holds for all $x \in \mathbb{R}$ and $\psi_s \in H^2_{loc}(\mathbb{R})$
We choose a function $\eta \in H^2(\mathbb{R})$ such that

$$\eta(x) = 1 \text{ for } |x| \le \frac{1}{4}, \quad \eta(x) = 0 \text{ for } |x| \ge \frac{1}{2},$$

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

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

Then,

$$\begin{aligned}
(A-\lambda I)u_l &= \sum_{j\in\mathbb{N}} \left[(-\frac{d^2}{dx^2} - \lambda) u_l|_{(x_j,x_{j+1})} \cdot \mathbb{1}_{(x_j,x_{j+1})} \right] \qquad (1.7)\\
&= \sum_{j\in\mathbb{N}} \left[\left(-\frac{d^2}{dx^2} - \lambda\right) \left(\eta\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})} \cdot \mathbb{1}_{(x_j,x_{j+1})} \right]\\
&= \sum_{j\in\mathbb{N}} \left[\eta\left(\frac{|\cdot|}{l}\right) \left(-\frac{d^2}{dx^2} - \lambda\right) \psi_s(\cdot,k)|_{(x_j,x_{j+1})} \cdot \mathbb{1}_{(x_j,x_{j+1})} \right]\\
&\quad - \frac{2}{l}\sum_{j\in\mathbb{N}} \left[\left(\eta'\left(\frac{|\cdot|}{l}\right)\psi_s'(\cdot,k)\right)\Big|_{(x_j,x_{j+1})} \cdot \mathbb{1}_{(x_j,x_{j+1})} \right]\\
&\quad - \frac{1}{l^2}\sum_{j\in\mathbb{N}} \left[\left(\eta''\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})} \cdot \mathbb{1}_{(x_j,x_{j+1})} \right]\\
&= \sum_{j\in\mathbb{N}} \left[\eta\left(\frac{|\cdot|}{l}\right) \left(-\frac{d^2}{dx^2} - \lambda\right) \psi_s(\cdot,k)|_{(x_j,x_{j+1})} \cdot \mathbb{1}_{(x_j,x_{j+1})} \right] + R
\end{aligned}$$

where R is a sum of products of derivatives (of order ≥ 1) of $\eta(\frac{|\cdot|}{l})$, and derivatives (of order ≤ 1) of $\psi_s(\cdot,k)$. Thus (note that $\psi_s(\cdot,k) \in H^2_{loc}(\mathbb{R})$), and the semi-periodic structure of $\psi_s(\cdot,k)$ implies

$$\|R\| \le \frac{c}{l}\|\psi_s(\cdot,k)\|_{H^1(K_l)} \le c\frac{1}{\sqrt{l}}, \tag{1.8}$$

with K_l denoting the ball in $\mathbb{R}$ with radius l, centered at x_0. Together with (1.6), (1.7) and (1.8), this gives

$$\|(A - \lambda I)u_l\| \leq \frac{c}{\sqrt{l}}$$

Again, by the semiperiodicity of $\psi_s(\cdot, k)$,

$$\|u_l\| \geq c\|\psi_s(\cdot, k)\| \geq c\sqrt{l}$$

with $c > 0$. We obtain therefore

$$\frac{1}{\|u_l\|}\|(A - \lambda I)u_l\| \leq \frac{c}{l}$$

Because moreover $u_l \in D(A)$, this results in

$$\frac{1}{\|u_l\|}\|(A - \lambda I)u_l\| \to 0 \text{ as } l \to \infty$$

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

Theorem 1.3. $\sigma(A) \subset \bigcup_{s\in\mathbb{N}} I_s$.

Beweis. todo □

TODO Theorem 3.6.3.

2 Appendix

Theorem 2.1 (Lax-Milgram). *Let H be a real Hilbert space, with norm $\|\cdot\|$ and inner product $\langle\cdot,\cdot\rangle$ as well as the pairing of H with its dual space. Assume that*

$$B\colon H \times H \to R$$

is a bilinear mapping, for which there exist constant $\alpha, \beta > 0$ such that

$$|B[u,v]| \leq \alpha\|u\|\|v\| \quad (u, v \in H)$$

and

$$\beta\|u\|^2 \leq B[u,u] \quad (u \in H)$$

Finally, let $f\colon H \to \mathbb{R}$ be a bounded linear functional on H.

Then there exists a unique element $u \in H$ such that

$$B[u,v] = \langle f, v\rangle$$

for all $v \in H$.

Beweis. For each fixed element $u \in H$, the mapping $v \mapsto B[u,v]$ is a bounded linear functional on H; whence the Riesz' Representation Theorem asserts the existence of a unique element $w \in H$ satisfying

$$B[u,v] = \langle w, v\rangle \tag{2.1}$$

Let us write $Au = w$ whenever (2.1) holds; so that

$$B[u,v] = \langle Au, v\rangle \quad (u, v \in H)$$

We first claim $A\colon H \to H$ is a bounded linear operator. Indeed if $\lambda_1, \lambda_2 \in \mathbb{R}$ and $u_1, u_2 \in H$, we see for each $v \in H$ that

$$\begin{aligned}\langle A(\lambda_1 u_1 + \lambda_2 u_2), v\rangle &= B[\lambda_1 u_1 + \lambda_2 u_2, v], \text{ (by (2.1))}\\ &= \lambda_1 B[u_1, v] + \lambda_2 B u_2, v]\\ &= \lambda_1\langle Au_1, v\rangle + \lambda_2\langle Au_2, v\rangle, \text{ (by (2.1) again)}\\ &= \langle \lambda_1 Au_1 + \langle_2 Au_2, v\rangle.\end{aligned}$$

This equality obtains for each $v \in H$, and so A is linear. Furthermore

$$\|Au\|^2 = \langle Au, Au\rangle = B[u, Au] \leq \alpha\|u\|\|Au\|.$$

Consequently $\|Au\| \leq \alpha\|u\|$ for all $u \in H$, and so A is bounded.

Next we assert

$$\begin{cases} A \text{ is one-to-one, and} \\ R(A), \text{ the range of } A, \text{ is close in } H. \end{cases} \tag{2.2}$$

To prove this, let us compute

$$\beta\|u\|^2 \leq B[u, u] = \langle Au, u\rangle \leq \|Au\|\|u\|$$

Hence $\beta\|u\| \leq \|Au\|$. This inequality easily implies (2.2).
We demonstrate now

$$R(A) = H \tag{2.3}$$

For if not, then, since $R(A)$ is closed, there would exist a nonzero element $w \in H$ with $w \in R(A)^\perp$. But this fact in turn implies the contradiction $\beta\|w\|^2 \leq B[w, w] = \langle Aw, w\rangle = 0$.
Next, we observe once more from the Riesz' Representation Theorem that

$$\langle f, v\rangle = \langle w, v\rangle \text{ for all } v \in H$$

for some element $w \in H$. We then utilise (2.2) and (2.3) to find $u \in H$ satisfying $Au = w$. Then

$$B[u, v] = \langle Au, v\rangle = \langle w, v\rangle = \langle f, v\rangle (v \in H)$$

and this is the claim.

Finally, we show there is at most one element $u \in H$ verifying the claim. For if both $B[u, v] = \langle f, v\rangle$ and $B[\tilde{u}, v] = \langle f, v\rangle$, then $B[u - \tilde{u}, v] = 0$ $(v \in H)$. We set $v = u - \tilde{u}$ to find $\beta\|u - \tilde{u}\|^2 \leq B[u - \tilde{u}, u - \tilde{u}] = 0$. □

Theorem 2.2 (Sobolev Embedding)**.**

$$H^1[0, 1] \subset C[0, 1].$$

Beweis. Prove that the H^1 norm dominates the C norm, namely, sup-norm, on $C_c^\infty[0,1]$. First, for $0 \leq x \leq y \leq 1$, the difference between maximum and minimum values of $f \in C_c^\infty[0,1]$ is constrained:

$$|f(y)-f(x)| = |\int_x^y f'(t)dt| \leq \left(\int_0^1 |f'(t)|^2 dt\right)^{1/2} \cdot |x-y|^{\frac{1}{2}} = \|f'\|_{L^2} \cdot |x-y|^{\frac{1}{2}}$$

Let $y \in [0,1]$ be such that $|f(y) = \min_x |f(x)|$. Then, using this inequality,

$$\begin{aligned} |f(x)| &\leq |f(y)| + |f(x) - f(y)| \\ &\leq \int_0^1 |f(t)dt + |f(x) - f(y)| \\ &\leq \|f\| + \|f'\| \ll 2\left(\|f\|^2 + \|f'\|^2\right)^{1/2} = 2\|f\|_{H^1} \end{aligned}$$

Thus, on $C_c^\infty[0,1]$ the H^1 norm dominates the sup-norm and therefore this comparison holds on the H^1 completion $H^1[0,1]$, and $H^1[0,1] \subset C[0,1]$. $\square$