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The Dislocation Problem in Hilbert Spaces

Vorlesungsskript
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Contents

Chapter 1

The periodic dislocation problem on $\mathbb{R}$, $\mathbb{R} \times [0, 1]$ and $\mathbb{R}^2$

1.1 Introduction

In solid state physics, one first studies crystallized matter with a perfectly regular atomic structure where the atoms are located on a periodic lattice. However, most crystals are not perfectly periodic; in fact, the regular pattern of atoms may be disturbed by various defects which fall into two main classes:

(i) defects which leave the lattice unchanged (like impurities or vacancies)

(ii) "geometric" defects of the lattice itself which may involve translations and rotation of portions of the lattice. Lattice dislocations occur, in particular, at grain boundaries in alloys. The models presented here are deterministic but may be generalized to include randomness.

Many of the geometric defects mentioned above are accessible to mathematical analysis only after some idealization which leads to the following type of problem: there is a periodic potential $V\colon \mathbb{R}^d \to \mathbb{R}$ with period lattice $\mathbb{Z}^d$ and a Euclidean transformation $T\colon \mathbb{R}^d \to \mathbb{R}^d$ such that the potential coincides with V in the half-space $\{x \in \mathbb{R}^d \mid x_1 \geq 0\}$ and with $V \circ T$ in $\{x_1 < 0\}$. In the simplest cases T is translation in the direction of one of the coordinate axes, with again two main subcases: translation orthogonal to the hyperplane $\{x_1 = 0\}$ or translations that keep the x_1-coordinate fixed.

The one-dimensional dislocation problem is particularly simple: Let $V : \mathbb{R} \to \mathbb{R}$ be a periodic potential with period 1 and let

$$W_t(x) := \begin{cases} V(x), & x \geq 0, \\ V(x+t), & x < 0, \end{cases} \tag{1.1}$$

for $t \in [0,1]$. The (self-adjoint) operator $H_t := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + W_t$ is called the *dislocation operator*, t the *dislocation parameter*. We are interested in the spectral properties of the operators H_t. We will see that the essential spectrum of H_t does not depend on t for $0 \le t \le 1$; also H_t cannot have any embedded eigenvalues. Precisely, $\sigma_{\mathrm{ess}}(H_t)$ has a band-gap-structure. For $0 < t < 1$, the operators H_t may have bound states (discrete eigenvalues) located in the gaps of the essential spectrum. We intend to give a systematic treatment of regularity properties of the eigenvalue "branches"; in particular, we show that the eigenvalue branches are Lipschitz-continuous if V is (locally) of bounded variation.

1.2 The Kato class

Let h_0 denote the (unique) self-adjoint extension of $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ defined on $C_c^\infty(\mathbb{R})$. Our basic class of potentials is given by

$$\mathcal{P} := \{V \in L_{1,\mathrm{loc}}(\mathbb{R},\mathbb{R});\ \forall x \in \mathbb{R} \colon V(x+1) = V(x)\}\,. \tag{1.2}$$

Potentials $V \in \mathcal{P}$ belong to the class $L_{1,\mathrm{loc,unif}}(\mathbb{R})$ which coincides with the Kato-class on the real line; in the subsequent estimates we will use

$$\|V\|_{1,\mathrm{loc,unif}} := \sup_{y\in\mathbb{R}} \int_y^{y+1} |V(x)|\,\mathrm{d}x \tag{1.3}$$

as a natural norm on $L_{1,\mathrm{loc,unif}}(\mathbb{R})$. In particular, any $V \in \mathcal{P}$ has relative form-bound zero with respect to h_0 and thus the form-sum H of h_0 and $V \in \mathcal{P}$ is well defined, cf. [CFrKS]. For $V \in \mathcal{P}$ given, we define the dislocation potentials W_t as in (1.1), for $0 \le t \le 1$; as before, the form-sum H_t of h_0 and W_t is well defined.

We intend to discuss some basic facts concerning continuity and regularity of the eigenvalue branches for the one-dimensional dislocation problem. We will see that for potentials belonging to the class $\mathcal{P}$, the eigenvalues are continuous functions of the dislocation parameter t.

Definition 1.1. A family of functions $J_a \colon \mathbb{R}^d \to \mathbb{R}$, $a \in A$, indexed by a set A is called a *partition of unity* if

(i) $0 \le J_a(x) \le 1$ for all $x \in \mathbb{R}^d$,

(ii) $\sum_{a\in A} J_a^2(x) = 1$ for all $x \in \mathbb{R}^d$,

(iii) (J_a) is locally finite, i.e. on any compact set K we have that $J_a = 0$ for all but finitely many $a \in A$,

(iv) $J_a \in C^\infty(\mathbb{R}^d)$,

(v) $\sup\left\{x \in \mathbb{R}^d;\ \sum_{a\in A} |\nabla J_a(x)|^2\right\} < \infty$.

Theorem 1.2 (IMS localization formula). *Let $(J_a)_{a\in A}$ be a partition of unity and let $H = h_0 + V$ for a potential V belonging to the Kato class. Then:*

$$H = \sum_{a\in A} J_a H J_a - \sum_{a\in A} |\nabla J_a|^2.$$

Proof. Exercise 2. □

Remark 1.3. The term $\sum_{a\in A} |\nabla J_a|^2$ is called the localization error.

Lemma 1.4. *For any $\varepsilon > 0$ there exists a constant $C_\varepsilon \geq 0$ such that for any $V \in L_{1,\mathrm{loc,unif}}(\mathbb{R})$ we have*

$$\int_{\mathbb{R}} |V|\,|\varphi|^2 \,\mathrm{d}x \leq \|V\|_{1,\mathrm{loc,unif}} \left(\varepsilon \|\varphi'\|^2 + C_\varepsilon \|\varphi\|^2\right), \qquad \varphi \in \mathcal{H}^1(\mathbb{R}). \tag{1.4}$$

Proof. For $f \in C_c^\infty(\mathbb{R})$ with support contained in $(0,\varepsilon)$ we have $\|f\|_\infty \leq \sqrt{\varepsilon}\,\|f'\|$. Let $(\zeta_n)_{n\in\mathbb{N}}$ denote a (locally finite) partition of unity on the real line with the properties: supp $\zeta_1 \subset (0,\varepsilon)$, each ζ_n is a translate of ζ_1, $M := \sup_{x\in\mathbb{R}} \sum_{n\in\mathbb{N}} |\zeta_n'(x)|^2$ is finite and $\sum_{n\in\mathbb{N}} \zeta_n^2(x) = 1$ for all $x \in \mathbb{R}$. By the IMS localization formula, we have for any $\varphi \in C_c^\infty(\mathbb{R})$,

$$\|\varphi'\|^2 = \langle -\varphi'', \varphi\rangle = \sum_{n=1}^\infty \|(\zeta_n\varphi)'\|^2 - \sum_{n=1}^\infty \|\zeta_n'\varphi\|^2 \geq \sum_{n=1}^\infty \|(\zeta_n\varphi)'\|^2 - M\|\varphi\|^2,$$

so that

$$\begin{aligned}\int |V(x)||\varphi(x)|^2 \,\mathrm{d}x &\leq \sum_{n=1}^\infty \|\zeta_n\varphi\|_\infty^2 \int_{\mathrm{supp}\ \zeta_n} |V(x)|\,\mathrm{d}x \\ &\leq \varepsilon\left(\|\varphi'\|^2 + M\|\varphi\|^2\right)\|V\|_{1,\mathrm{loc,unif}}.\end{aligned}$$

The general case follows by approximation and Fatou's lemma. □

For $V \in \mathcal{P}$, the function

$$\vartheta_V(s) := \int_0^1 |V(x+s) - V(x)|\,\mathrm{d}x, \qquad 0 \leq s \leq 1, \tag{1.5}$$

is continuous and $\vartheta_V(s) \to 0$, as $s \to 0$. Furthermore, for W_t is as (1.1), we have $\|W_t - W_{t'}\|_{1,\mathrm{loc,unif}} = \vartheta_V(t-t')$. This leads to the following lemma.

Lemma 1.5. *Let $V \in \mathcal{P}$, $E_0 \in \mathbb{R}\setminus\sigma(H_{t_0})$, and write $\varepsilon_0 := \mathrm{dist}(E_0, \sigma(H_{t_0}))$. Then there is $\tau_0 > 0$ such that H_t has no spectrum in $(E_0-\varepsilon_0/2, E_0+\varepsilon_0/2)$ for $|t-t_0| < \tau_0$. Furthermore, there exists a constant $C \geq 0$ such that for some $\tau_1 \in (0,\tau_0)$*

$$\left\|(H_t - E_0)^{-1} - (H_{t_0} - E_0)^{-1}\right\| \leq C\vartheta_V(t-t_0), \qquad |t-t_0| < \tau_1. \tag{1.6}$$

Proof. Without loss of generality we may assume that $V \geq 1$. Let $\mathbf{h}_t$ denote the quadratic form associated with H_t. Applying Lemma 1.4 (with $\varepsilon := 1$) we see that

$$|\mathbf{h}_{t_0}[u] - \mathbf{h}_t[u]| \leq \int_{\mathbb{R}} |W_t - W_{t_0}|\, |u|^2 \,\mathrm{d}x \leq C_1 \vartheta_V(t - t_0)\mathbf{h}_{t_0}[u], \qquad u \in \mathcal{H}^1(\mathbb{R}),$$

with some constant C_1. The desired result now follows by [K; Thm. VI-3.9]. □

We therefore see that $H_{t_n} \to H_{t_0}$ in the sense of norm resolvent convergence if $t_0 \in [0,1]$, $(t_n)_{n\in\mathbb{N}} \subset [0,1]$ and $t_n \to t_0$. By standard arguments, this implies that the discrete eigenvalues of H_t depend continuously on t.

Let

$$\mathcal{P}_\alpha := \{V \in \mathcal{P} \mid \exists C \geq 0\colon \vartheta_V(s) \leq Cs^\alpha, \forall 0 < s \leq 1\}, \tag{1.7}$$

where $0 < \alpha \leq 1$. The class $\mathcal{P}_\alpha$ consists of all periodic functions $V \in \mathcal{P}$ which are (locally) α-Hölder-continuous in the L_1-mean; for $\alpha = 1$ this is a Lipschitz-condition in the L_1-mean. The class $\mathcal{P}_1$ is of particular practical importance since it contains the periodic step functions. We can show that $\mathcal{P}_1$ coincides with the class of periodic functions on the real line which are locally of bounded variation.

Proposition 1.6. *Let $BV_{\mathrm{loc}}(\mathbb{R})$ denote the space of real-valued functions which are of bounded variation over any compact subset of the real line.*

Then $\mathcal{P}_1 = \mathcal{P} \cap BV_{\mathrm{loc}}(\mathbb{R})$.

It is easy to see that any $V \in \mathcal{P} \cap BV_{\mathrm{loc}}(\mathbb{R})$ belongs to $\mathcal{P}_1$: certainly, any $V \in \mathcal{P}$ which is monotonic over $[0,1]$ is an element of $\mathcal{P}_1$ and any function of bounded variation can be written as the difference of two monotonic functions.

The converse direction is established by the following lemma.

Lemma 1.7. *Let $f \in L_{1,\mathrm{loc}}(\mathbb{R},\mathbb{R})$ be periodic with period 1 and suppose that there are $c \geq 0$, $\varepsilon > 0$ such that*

$$\int_0^1 |f(x+t) - f(x)| \,\mathrm{d}x \leq ct, \qquad \forall 0 < t < \varepsilon. \tag{1.8}$$

Consider f as a function in $L_1(\mathbb{T})$, with $\mathbb{T}$ denoting the one-dimensional torus.

We then have: the distributional derivative ∂f is a (signed) Borel-measure μ on $\mathbb{T}$ and there is a number $a \in \mathbb{R}$ such that $f(x) = a + \mu([0,x))$, a.e. in $[0,1) \simeq \mathbb{T}$. In particular, f has a left-continuous representative of bounded variation.

Proof. Defining $\eta\colon C^1(\mathbb{T}) \to \mathbb{R}$ by

$$\eta(\varphi) := -\int_0^1 \varphi' f \,\mathrm{d}x,$$

we may compute

$$-\int_0^1 \varphi' f \,\mathrm{d}x = \lim_{t\to 0} \int_0^1 \frac{1}{t}(\varphi(x-t) - \varphi(x)) f(x) \,\mathrm{d}x$$
$$= \lim_{t\to 0} \int_0^1 \varphi(x) \frac{1}{t}(f(x+t) - f(x)) \,\mathrm{d}x,$$

and the assumption yields the estimate $|\eta(\varphi)| \le c \|\varphi\|_\infty$. Since $C^1(\mathbb{T})$ is dense in $C(\mathbb{T})$, the functional η has a unique continuous extension to all of $C(\mathbb{T})$; we denote the extension by the same symbol η. By the Riesz representation theorem there is a measure μ such that $\eta(\varphi) = \int \varphi \,\mathrm{d}\mu$ for all $\varphi \in C(\mathbb{T})$. Furthermore, for $\varphi \in C^1(\mathbb{T})$ we have $-\int_0^1 \varphi' f \,\mathrm{d}x = \int_0^1 \varphi \,\mathrm{d}\mu$, and we see that $\mu = \partial f$ on $\mathbb{T}$ in the distributional sense. The choice $\varphi := 1$ yields $\int_{\mathbb{T}} \mathrm{d}\mu = -\int_0^1 \varphi' f \,\mathrm{d}x = 0$ and the function $\tilde f(x) := \mu([0,x))$ satisfies $\partial \tilde f = \mu$. This is easy to check: for $\varphi \in C^1(\mathbb{T})$ we have

$$\int \tilde f \varphi' \,\mathrm{d}x = \int_0^1 \int_{0\le y<x} \mathrm{d}\mu(y) \varphi'(x) \,\mathrm{d}x$$
$$= \int_{0\le y<1} \int_y^1 \varphi'(x) \,\mathrm{d}x \,\mathrm{d}\mu(y) = -\int_{[0,1)} \varphi(y) \,\mathrm{d}\mu(y).$$

We therefore see that $\partial(f - \tilde f) = 0$; hence there is some a such that $f - \tilde f = a$. $\square$

1.3 Eigenvalues in spectral gaps

We begin with some well-known results pertaining to the spectrum of $H = H_0$. As explained in [E, RS-IV], we have

$$\sigma(H) = \sigma_{\mathrm{ess}}(H) = \cup_{k=1}^\infty [\gamma_k, \gamma_k'], \tag{1.9}$$

where the γ_k and γ_k' satisfy $\gamma_k < \gamma_k' \le \gamma_{k+1}$, for all $k \in \mathbb{N}$, and $\gamma_k \to \infty$ as $k \to \infty$. Moreover, the spectrum of H is purely absolutely continuous. The intervals $[\gamma_k, \gamma_k']$ are called the *spectral bands* of H. The open intervals $\Gamma_k := (\gamma_k', \gamma_{k+1})$ are the *spectral gaps* of H; we say the k-th gap is *open* or *non-degenerate* if $\gamma_{k+1} > \gamma_k'$.

In order to determine the essential spectrum of H_t for $0 < t < 1$, we introduce Dirichlet boundary conditions at $x = 0$ for the operator H_0 and at $x = 0$ and $x = -t$ for H_t to obtain the operators

$$H_D = H^- \oplus H^+, \quad H_{t,D} = H_t^- \oplus H_{(-t,0)} \oplus H^+, \tag{1.10}$$

where $H^\pm$ acts in $\mathbb{R}^\pm$ with a Dirichlet boundary condition at 0, H_t^- in $(-\infty, -t)$ with Dirichlet boundary condition at $-t$ and $H_{(-t,0)}$ in $(-t, 0)$ with Dirichlet boundary conditions at $-t$ and 0. Since $H_{(-t,0)}$ has purely discrete spectrum and since the operators H_t^- and H^- are unitarily equivalent, we conclude that $\sigma_{\mathrm{ess}}(H_D) = \sigma_{\mathrm{ess}}(H_{t,D})$.

It is well known that decoupling by (a finite number of) Dirichlet boundary conditions leads to compact perturbations of the corresponding resolvents (in fact, perturbations of finite rank) and thus Weyl's essential spectrum theorem yields $\sigma_{\text{ess}}(H_D) = \sigma_{\text{ess}}(H)$ and $\sigma_{\text{ess}}(H_{t,D}) = \sigma_{\text{ess}}(H_t)$.

In addition to the essential spectrum, the operators H_t may have discrete eigenvalues below the infimum of the essential spectrum and inside any (non-degenerate) gap, for $t \in (0,1)$; these eigenvalues are simple. We provide a complete and precise picture concerning the eigenvalue branches in the following lemma saying that the discrete eigenvalues of H_t inside a given gap Γ_k of H can be described by an (at most) countable, locally finite family of continuous functions, defined on suitable subintervals of $[0,1]$.

Lemma 1.8. *Let $k \in \mathbb{N}$ and suppose that the gap Γ_k of H is open, i.e., $\gamma_k' < \gamma_{k+1}$. Then there is a (finite or countable) family of continuous functions $f_j\colon (\alpha_j, \beta_j) \to \Gamma_k$, where $0 \le \alpha_j < \beta_j \le 1$, with the following properties:*

(i) $f_j(t)$ is an eigenvalue of H_t, for all $\alpha_j < t < \beta_j$ and for all j. Conversely, for any $t \in (0,1)$ and any eigenvalue $E \in \Gamma_k$ of H_t there is a unique index j such that $f_j(t) = E$.

(ii) As $t \downarrow \alpha_j$ (or $t \uparrow \beta_j$), the limit of $f_j(t)$ exists and belongs to the set $\{\gamma_k', \gamma_{k+1}\}$.

(iii) For all but a finite number of indices j the range of f_j does not intersect a given compact subinterval $[a', b'] \subset \Gamma_k$.

Proof. We consider $t \in \mathbb{T}$, the flat one-dimensional torus, and we denote the spectral gap by (a,b). Let $[a',b'] \subset (a,b)$.

(1) Let $(\eta, \tau) \in (a,b) \times \mathbb{T}$. Since $\sigma(H_\tau) \cap (a,b)$ is a discrete set, and since $\sigma(H_t)$ depends continuously on t, there is a neighborhood $U_{\eta,\tau} \subset (a,b) \times \mathbb{T}$ of (η,τ) of the form $U_{\eta,\tau} = (\eta_1, \eta_2) \times (\tau_1, \tau_2)$ belonging to either of the two following types:
Type (1): For $\tau_1 < t < \tau_2$ we have $\sigma(H_t) \cap (\eta_1, \eta_2) = \emptyset$.
Type (2): η is an eigenvalue of H_τ and there is a continuous function $f\colon (\tau_1, \tau_2) \to (\eta_1, \eta_2)$ such that $f(t)$ is an eigenvalue of H_t; H_t has no further eigenvalues in (η_1, η_2), for $\tau_1 < t < \tau_2$.
Now the family $\{U_{\eta,\tau};\ (\eta,\tau) \in (a,b) \times \mathbb{T}\}$ is an open cover of $(a,b) \times \mathbb{T}$ and there exists a finite selection $\{U_{\eta_i,\tau_i}\}_{i=1,\dots,N}$ such that

$$[a',b'] \times \mathbb{T} \subset \cup_{i=1}^N U_{\eta_i,\tau_i}.$$

As a first consequence, we see that there is at most a finite number of functions that describe the spectrum of H_t in the open set $\cup_{i=1}^N U_{\eta_i,\tau_i} \supset [a',b'] \times \mathbb{T}$.

(2) Suppose that $(\eta,\tau) \in (a,b) \times \mathbb{T}$ is such that $\eta \in \sigma(H_\tau)$ and let $f\colon (\tau_1,\tau_2) \to (\eta_1,\eta_2)$ as above. Consider a sequence $(t_j)_{j\in\mathbb{N}} \subset (\tau_1, \tau_2)$ with $t_j \to \tau_1$. We can find a subsequence $(t_{j_k})_{k\in\mathbb{N}}$ such that $f(t_{j_k}) \to \bar{\eta}$ for some $\bar{\eta} \in [\eta_1, \eta_2]$. It is easy to see

that $\bar{\eta} \in \sigma(H_{\tau_1})$. If $\bar{\eta} \in (a,b)$ the point $(\bar{\eta}, \tau_1)$ has a neighborhood $U_{\bar{\eta},\tau_1}$ of type (2) and we can extend the domain of definition of f beyond τ_1. It follows that there exist a maximal open interval $(\alpha, \beta) \subset (0,1)$ and a (unique) continuous extension $\tilde{f}\colon (\alpha,\beta) \to (a,b)$ of f such that $\tilde{f}(t)$ is an eigenvalue of H_t for all $t \in (\alpha,\beta)$.

(3) It remains to show that $\tilde{f}(t)$ converges to a band edge as $t \downarrow \alpha$ and as $t \uparrow \beta$. By the same argument as above, we find that any sequence $(t_j)_{j\in\mathbb{N}} \subset (\alpha,\beta)$ satisfying $t_j \to \alpha$ has a subsequence $(t_{j_k})_{k\in\mathbb{N}}$ such that $\tilde{f}(t_{j_k}) \to \bar{\eta}$ for some $\bar{\eta} \in [a,b]$. Here $\bar{\eta} \notin (a,b)$ because otherwise we could again extend the domain of definition of $\tilde{f}$ beyond α, contradicting the maximality property of the interval (α,β).

Suppose there are sequences $(t_j)_{j\in\mathbb{N}}, (s_j)_{j\in\mathbb{N}} \subset (\alpha,\beta)$ such that $t_j \to \alpha$ and $s_j \to \alpha$ and $\tilde{f}(t_j) \to a$ while $\tilde{f}(s_j) \to b$ as $j \to \infty$. Then for any $\eta' \in (a,b)$ there is a sequence $(r_j)_{j\in\mathbb{N}} \subset (\alpha,\beta)$ such that $r_j \to \alpha$ and $\tilde{f}(r_j) \to \eta'$, whence $\eta' \in \sigma(H_\alpha)$. This would imply that $(a,b) \subset \sigma(H_\alpha)$, which is impossible. □

We next turn our attention to the question of Lipschitz-continuity of the functions f_j in Lemma 1.8. Recall that the class $\mathcal{P}_1$ consists of all periodic functions $V \in \mathcal{P}$ which are (locally) Lipschitz-continuous in the L_1-mean.

Proposition 1.9. *For $V \in \mathcal{P}_1$, let (a,b) denote any of the gaps Γ_k of H and let $f_j\colon (\alpha_j,\beta_j) \to (a,b)$ be as in Lemma 1.8. Then the functions f_j are uniformly Lipschitz-continuous. More precisely, for each gap Γ_k there exists a constant $C_k \geq 0$ such that for all j*

$$|f_j(t) - f_j(t')| \leq C_k|t-t'|, \qquad \alpha_j \leq t, t' \leq \beta_j.$$

Proof. Exercise 3. □

Remark 1.10.

(1) We can also obtain the following result on Hölder-continuity: If $0 < \alpha < 1$ and $V \in \mathcal{P}_\alpha$, then each of the functions $f_j\colon (\alpha_j,\beta_j) \to (a,b)$ is locally uniformly Hölder-continuous (as defined in [GT]), i.e., for any compact subset $[\alpha_j', \beta_j'] \subset (\alpha_j,\beta_j)$ there is a constant $C = C(j, \alpha_j', \beta_j')$ such that $|f_j(t) - f_j(t')| \leq C|t-t'|^\alpha$, for all $t, t' \in [\alpha_j', \beta_j']$. Note that our method does not necessarily yield a uniform constant for the whole interval (α_j,β_j), much less a constant that would be uniform for all j.

(2) For analytic potentials V, it is shown in [K1] that the eigenvalue branches f_j in Lemma 1.8 depend analytically on t. This is a simple consequence of the fact that, for real analytic V, the H_t form a holomorphic family of self-adjoint operators in the sense of Kato. In [K2], the author proves that the f_j are squares of W_2^1-functions near the gap edges if the potential is in $L_2(\mathbb{T})$.

1.4 A spectral shift function

It is our aim in this section to show that at least k eigenvalues move from the upper to the lower edge of the k-th gap as the dislocation parameter ranges from 0 to 1. Using the notation of Lemma 1.8 and writing $f_i(\alpha_i) \coloneqq \lim_{t\downarrow\alpha_i} f_i(t)$, $f_i(\beta_i) \coloneqq \lim_{t\uparrow\beta_i} f_i(t)$, we now define

$$\mathcal{N}_k \coloneqq \#\{i;\ f_i(\alpha_i) = \gamma_{k+1},\ f_i(\beta_i) = \gamma_k'\} - \#\{i;\ f_i(\alpha_i) = \gamma_k',\ f_i(\beta_i) = \gamma_{k+1}\}. \quad (1.11)$$

Thus $\mathcal{N}_k$ is precisely the number of eigenvalue branches of H_t that cross the k-th gap moving from the upper to the lower edge minus the number crossing from the lower to the upper edge. Put differently, $\mathcal{N}_k$ is the spectral multiplicity which *effectively* crosses the gap Γ_k in downwards direction as t increases from 0 to 1.

Our main result in this section says that $\mathcal{N}_k = k$, provided the k-th gap is open:

Theorem 1.11. *Let $V \in \mathcal{P}$ and suppose that the k-th spectral gap of H is open, i.e., $\gamma_k' < \gamma_{k+1}$. Then $\mathcal{N}_k = k$.*

Again, the results obtained by Korotyaev in [K1, K2] are more detailed; e.g., it is shown that, for any $t \in (0,1)$, the dislocation operator H_t has two unique states (an eigenvalue and a resonance) in any given gap of the periodic problem. On the other hand, our variational arguments are more flexible and allow an extension to higher dimensions, as will be seen in the sequel. In this sense, the importance of this section lies in testing our approach in the simplest possible case.

The main idea of our proof goes as follows: consider a sequence of approximations on intervals $(-n-t, n)$ with associated operators $H_{n,t} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + W_t$ with periodic boundary conditions. We first observe that the gap Γ_k is free of eigenvalues of $H_{n,0}$ and $H_{n,1}$ since both operators are obtained by restricting a periodic operator on the real line to some interval of length equal to an entire multiple of the period, with periodic boundary conditions. Second, the operators $H_{n,t}$ have purely discrete spectrum and it follows from Floquet theory (cf. [E, RS-IV]) that $H_{n,0}$ has precisely $2n$ eigenvalues in each band while $H_{n,1}$ has precisely $2n+1$ eigenvalues in each band. As a consequence, effectively k eigenvalues of $H_{n,t}$ must cross any fixed $E \in \Gamma_k$ as t goes from 0 to 1. To obtain the result of Theorem 1.11 we only have to take the limit $n \to \infty$. Here we employ several technical lemmas. In the first one, we show that the eigenvalues of the family $H_{n,t}$ depend continuously on the dislocation parameter.

Lemma 1.12. *The eigenvalues of $H_{n,t}$ depend continuously on $t \in [0,1]$.*

Proof. Exercise 4. □

The next lemma is to establish a connection between the spectra of H_t and $H_{n,t}$ for $0 \le t \le 1$ and n large. In the proof and henceforth, we will make use of the following cut-off functions (see also Exercise 1): We pick some $\varphi \in C_c^\infty(-2,2)$ with

$0 \le \varphi \le 1$ and $\varphi(x) = 1$ for $|x| \le 1$. For $k \in (0,\infty)$ we then define $\varphi_k(x) := \varphi(x/k)$ so that supp $\varphi_k \subset (-2k, 2k)$, $\varphi_k(x) = 1$ for $|x| \le k$, $|\varphi_k'(x)| \le Ck^{-1}$ and $|\varphi_k''(x)| \le Ck^{-2}$. Finally, we let $\psi_k := 1 - \varphi_k$. For any self-adjoint operator T we denote the spectral projection associated with an interval $I \subset \mathbb{R}$ by $P_I(T)$ and we write dim $P_I(T)$ to denote the dimension of the range of the projection $P_I(T)$.

Lemma 1.13. *Let $k \in \mathbb{N}$ with $\Gamma_k \neq \emptyset$. Let $t \in (0,1)$ and suppose that $\eta_1 < \eta_2 \in \Gamma_k$ are such that $\eta_1, \eta_2 \notin \sigma(H_t)$. Then there is an $n_0 \in \mathbb{N}$ such that $\eta_1, \eta_2 \notin \sigma(H_{n,t})$ for $n \ge n_0$, and*

$$\dim P_{(\eta_1,\eta_2)}(H_t) = \dim P_{(\eta_1,\eta_2)}(H_{n,t}), \qquad n \ge n_0. \tag{1.12}$$

Proof. In the subsequent calculations, we always take $k := n/4$, for $n \in \mathbb{N}$.

(1) Let $E \in (\eta_1, \eta_2) \cap \sigma(H_t)$ with associated normalized eigenfunction u. Then $u_k := \varphi_k u \in D(H_{n,t})$, $H_{n,t} u_k = H_t u_k$ and $\|u_k\| \to 1$ as $n \to \infty$. Since

$$\|H_{n,t} u_k - E u_k\| \le 2 \cdot \|\varphi_k'\|_\infty \|u'\| + \|\varphi_k''\|_\infty \|u\|, \tag{1.13}$$

it is now easy to conclude that dim $P_{(\eta_1,\eta_2)}(H_{n,t}) \ge$ dim $P_{(\eta_1,\eta_2)}(H_t)$ for n large.

(2) We next assume for a contradiction that $\eta \in \Gamma_k$ satisfies $\eta \in \sigma(H_{n,t})$ for infinitely many $n \in \mathbb{N}$. Then there is a subsequence $(n_j)_{j\in\mathbb{N}} \subset \mathbb{N}$ s.th. $\eta \in \sigma(H_{n_j,t})$; we let $u_{n_j,t} \in D(H_{n_j,t})$ denote a normalized eigenfunction and set

$$v_{1,n_j} := \varphi_{k_j} u_{n_j,t}, \qquad v_{2,n_j} := \psi_{k_j} u_{n_j,t}, \tag{1.14}$$

so that $v_{1,n_j} \in D(H_t)$ and $\left\|(H_t - \eta) v_{1,n_j}\right\| \to 0$ as $j \to \infty$ by a similar estimate as in part (1) (and using a simple bound for $\left\|u_{n,t}'\right\|$ which follows from the fact that V has relative form-bound zero w.r.t. h_0.) Let us now show that $v_{2,n_j} \to 0$ (and hence $\left\|v_{1,n_j}\right\| \to 1$) as $j \to \infty$: The function

$$\tilde{v}_{2,n_j}(x) := \begin{cases} v_{2,n_j}(x), & x \ge 0, \\ v_{2,n_j}(x - t), & x < 0, \end{cases} \tag{1.15}$$

belongs to the domain of $H_{n_j,0}$ and $H_{n_j,0} \tilde{v}_{2,n_j} = [H_{n_j,t} v_{2,n_j}]^\sim$, where $[\cdot]^\sim$ is defined in analogy with (1.15). Since we also have $(H_{n_j,t} - \eta) v_{2,n_j} \to 0$, as $j \to \infty$, we see that $(H_{n_j,0} - \eta)\tilde{v}_{2,n_j} \to 0$. But $\mathrm{dist}(\eta, \sigma(H_{n,0})) \ge \delta_0 > 0$ for all n and the Spectral Theorem implies that $\left\|\tilde{v}_{2,n_j}\right\| \to 0$ as $j \to \infty$. We have thus shown that $\left\|v_{1,n_j}\right\| \to 1$ and $\left\|(H_t - \eta) v_{1,n_j}\right\| \to 0$ which implies that $\eta \in \sigma(H_t)$.

(3) It remains to show that dim $P_{(\eta_1,\eta_2)}(H_{n,t}) \le$ dim $P_{(\eta_1,\eta_2)}(H_t)$, for n large. The proof by contradiction follows the lines of part (2); instead of a sequence of functions u_{n_j} we work with an orthonormal system $u_{n_j}^{(1)}, \ldots, u_{n_j}^{(\ell)}$ of eigenfunctions where $\ell =$ dim $P_{(\eta_1,\eta_2)}(H_t + 1)$. We leave the details to the reader. □

Remark 1.14. In fact, using standard exponential decay estimates for resolvents of Schrödinger operators, cf. [S], it can be shown that the eigenvalues of H_t and $H_{n,t}$

in the gap Γ_k are exponentially close, for n large; e.g., if $E \in \sigma(H_t) \cap \Gamma_k$ for some $t \in (0,1)$, then there are constants $c \geq 0$ and $\alpha > 0$ s.th. the operators $H_{n,t}$ have an eigenvalue in $(E - c\mathrm{e}^{-\alpha n}, E + c\mathrm{e}^{-\alpha n})$, for n large.

The desired connection between the spectral flow for $(H_{n,t})_{0\leq t\leq 1}$ and $(H_t)_{0\leq t\leq 1}$ is obtained by applying Lemma 1.13 at suitable $t_i \in [0,1]$ and $\eta_{1,i} < \eta_{2,i} \in \Gamma_k$. We now construct an appropriate partition of the parameter interval $[0,1]$.

Lemma 1.15. *Let $k \in \mathbb{N}$ with $\Gamma_k \neq \emptyset$. Then there exists a partition $0 = t_0 < t_1 < \ldots < t_{K-1} < t_K = 1$ and there exist $E_j \in \Gamma_k$ and $n_0 \in \mathbb{N}$ such that*

$$E_j \notin \sigma(H_t) \cup \sigma(H_{n,t}), \qquad \forall t \in [t_{j-1}, t_j], \quad j = 1, \ldots, K, \quad n \geq n_0. \tag{1.16}$$

Proof. For any $t \in [0,1]$ there exists $\eta_t \in \Gamma_k$ such that $\eta_t \notin \sigma(H_t)$. Since the spectrum of H_t depends continuously on the parameter t there also exists $\varepsilon = \varepsilon_t > 0$ such that $\eta_t \notin \sigma(H_\tau)$ for all $\tau \in (t - \varepsilon_t, t + \varepsilon_t)$. By compactness, we can find a partition $(\tau_j)_{0\leq j\leq K}$ (with $\tau_0 = 0$, $\tau_K = 1$) such that the intervals $(\tau_j - \varepsilon_j, \tau_j + \varepsilon_j)$ cover $[0,1]$. Set $E_j \coloneqq \eta_{\tau_j}$. We next pick arbitrary points $t_j \in (\tau_j, \tau_j + \varepsilon_j) \cap (\tau_{j+1} - \varepsilon_{j+1}, \tau_{j+1})$, for $j = 1, \ldots, K-1$, set $t_0 = 0$, $t_K = 1$ and see that $E_j \notin \sigma(H_t)$ for $t_{j-1} \leq t \leq t_j$, $j = 1, \ldots, K$. By Lemma 1.13, using Lemma 1.12 combined with a simple compactness argument, we then find that we also have $E_j \notin \sigma(H_{n,t})$ for $t \in [t_{j-1}, t_j]$ and n large. □

We are now ready for the proof of Theorem 1.11.

Proof of Theorem 1.11 Let E_j be as in Lemma 1.15 and $\mathcal{N}_k$ as in (1.11). We fix some $\tilde{E} \in \Gamma_k$ such that $\tilde{E} > E_j$ for $j = 0, \ldots, K$ and $\tilde{E} \notin \sigma(H_{t_j}) \cup \sigma(H_{n,t_j})$ for $j = 0, \ldots, K$ and for all n large. It is then easy to see that

$$\mathcal{N}_k = \sum_{j=1}^{K} \Big(\dim\, P_{(E_j,\tilde{E})}(H_{t_j}) - \dim\, P_{(E_j,\tilde{E})}(H_{t_{j-1}}) \Big) \tag{1.17}$$

and that

$$\begin{aligned} \dim\, P_{(-\infty,\tilde{E})}(H_{n,1}) &- \dim\, P_{(-\infty,\tilde{E})}(H_{n,0}) \\ &= \sum_{j=1}^{K} \Big(\dim\, P_{(E_j,\tilde{E})}(H_{n,t_j}) - \dim\, P_{(E_j,\tilde{E})}(H_{n,t_{j-1}}) \Big) . \end{aligned} \tag{1.18}$$

The LHS of (1.18) equation equals k. Furthermore, by Lemma 1.13, we have

$$\dim\, P_{(E_j,\tilde{E})}(H_{t_j}) = \dim\, P_{(E_j,\tilde{E})}(H_{n,t_j}) \tag{1.19}$$

for all j and all n large, and the desired result follows. □

1.5 A one-dimensional periodic step potential

In this section, we study the one-dimensional 2π-periodic potential

$$V(x) := \begin{cases} -1, & x \in [0, \pi], \\ 1, & x \in (\pi, 2\pi). \end{cases} \tag{1.20}$$

(While the other parts of the script deal with 1-periodic potentials, we have preferred to work here with period 2π in order to keep the explicit calculations done by hand as simple as possible.) To obtain the band-gap structure of $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$, we compute the *discriminant function*

$$D(E) := \varphi_1(2\pi; E) + \varphi_2'(2\pi; E) = \operatorname{tr} \begin{pmatrix} \varphi_1(2\pi; E) & \varphi_1'(2\pi; E) \\ \varphi_2(2\pi; E) & \varphi_2'(2\pi; E) \end{pmatrix} \tag{1.21}$$

where $\varphi_1(\,\cdot\,; E)$ and $\varphi_2(\,\cdot\,; E)$ solve the equation

$$-u'' + (V - E)u = 0 \tag{1.22}$$

and satisfy the boundary conditions

$$\varphi_1(0; E) = \varphi_2'(0; E) = 1 \quad \text{and} \quad \varphi_1'(0; E) = \varphi_2(0; E) = 0. \tag{1.23}$$

The matrix $M(E)$ on the RHS of (1.21) is called the *monodromy matrix.* A simple computation shows that $[-1/2, 1/2] \subset \Gamma_1$, where Γ_1 is the first spectral gap of H (with numbering according to Floquet theory). Note that the gap edges of Γ_1 also equal the first eigenvalue in the (semi-)periodic eigenvalue problem for $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ in $L_2(0, 2\pi)$, cf., e.g., [E, CL].

As explained in [E, RS-IV], for any $E \notin \sigma(H)$, there are two solutions $\varphi_\pm(x; E) \in C^1(\mathbb{R})$, square integrable at $\pm\infty$, of (1.22); in fact, the functions $\varphi_\pm(x; E)$ are exponentially decaying at $\pm\infty$ and exponentially increasing at $\mp\infty$. In our example, the dislocation potential W_t for $t \in (0, 1)$ will produce a bound state at E if and only if the boundary conditions coming from $\varphi_+(0; E)$ and $\varphi_-(t; E)$ match up, i.e.,

$$\varphi_-(t; E) = \varphi_+(0; E) \quad \text{and} \quad \varphi_-'(t; E) = \varphi_+'(0; E). \tag{1.24}$$

An equivalent condition for (1.24) is the equality of the ratio functions $\frac{\varphi_-(t;E)}{\varphi_-'(t;E)}$ and $\frac{\varphi_+(0;E)}{\varphi_+'(0;E)}$. In Exerice 5, the Floquet solutions $\varphi_\pm$ are computed by solving the equation $-u'' + (V - E)u = 0$ for $x < 0$ and $x > 0$ and for E varying in $[-1/2, 1/2]$, assuming that $(u(0), u'(0))$ equals an appropriate eigenvector of $M(E)$. Note that, since $D(E) < -2$, both eigenvalues of $M(E)$ are negative and not equal to -1. Finally, the interval $[-1/2, 1/2]$ is divided into 100 subintervals of equal length and numerical values for t are computed with *Mathematica* such that

$$\left| \frac{\varphi_-(t; E)}{\varphi_-'(t; E)} - \frac{\varphi_+(0; E)}{\varphi_+'(0; E)} \right| < \varepsilon, \tag{1.25}$$

where the error $\varepsilon > 0$ is suitably small. This leads to the following plot of $t \mapsto E(t)$, see Fig. 1.1.

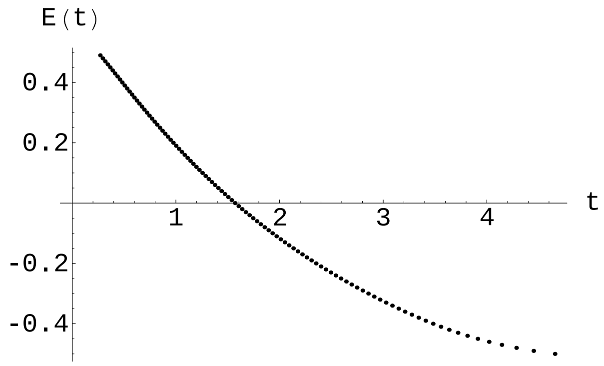

Figure 1.1: An eigenvalue branch of H_t in the first spectral gap.

References

[AADH] S Alama, M Avellanda, PA Deift, and R Hempel, *On the existence of eigenvalues of a divergence form operator $A+\lambda B$ in a gap of $\sigma(A)$*, Asymptotic Analysis **8** (1994), 311–344

[CFrKS] HL Cycon, RG Froese, W Kirsch, and B Simon, *Schrödinger Operators with Applications to Quantum Mechanics and Global Geometry*, Springer, New York, 1987

[CL] E Coddington and N Levinson, *Theory of Ordinary Differential Equations*, McGraw-Hill, New York, 1955

[DS] EB Davies and B Simon, *Scattering theory for systems with different spatial asymptotics on the left and right*, Commun. Math. Phys. **63** (1978), 277–301

[E] MSP Eastham, *The Spectral Theory of Periodic Differential Equations*, Scottish Academic Press, Edinburgh, London, 1973

[EKSchrS] H Englisch, W Kirsch, M Schröder, and B Simon, *Random Hamiltonians ergodic in all but one direction*, Commun. Math. Phys. **128** (1990), 613–625

[GT] D Gilbarg and NS Trudinger, *Elliptic Partial Differential Equations of Second Order*, Springer, New York, 1977

[H92] R Hempel, Eigenvalues in gaps and decoupling by Neumann boundary conditions, J. Math. Anal. Appl. **169** (1992), 229–259

[K] T Kato, *Perturbation Theory for Linear Operators*, Springer, New York, 1966

[K1] E Korotyaev, *Lattice dislocations in a 1-dimensional model*, Commun. Math. Phys. **213** (2000), 471–489

[K2] E Korotyaev, *Schrödinger operators with a junction of two 1-dimensional periodic potentials*, Asymptotic Anal. **45** (2005), 73–97

[KS] V Kostrykin and R Schrader, *Regularity of the surface density of states*, J. Funct. Anal. **187** (2001), 227–246

[RS-I] M Reed and B Simon, *Methods of Modern Mathematical Physics. Vol I. Analysis of Operators*, Revised and enlarged edition, Academic Press, New York, 1979

[RS-IV] M Reed and B Simon, Methods of Modern Mathematical Physics. Vol IV. Analysis of Operators, Academic Press, New York, 1978

[S] B Simon, *Schrödinger semigroups*, Bull. Amer. Math. Soc. **7** (1982), 447–526

[S78] B Simon, *A canonical decomposition for quadratic forms with applications to monotone convergence theorems,* J. Funct. Anal. **28** (1978), 267–273