GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

The Dislocation Problem in Hilbert Spaces

Vorlesungsskript
Sommersemester 2019

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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: $\operatorname{supp}\zeta_1 \subset (0,\varepsilon)$, 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

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

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 $\varepsilon_0 := \operatorname{dist}(E_0, \sigma(H_{t_0}))$. 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

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

and the assumption yields the estimate $|\eta(\varphi)| \leq c\,\|\varphi\|_\infty$. 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

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

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

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 $\gamma_k < \gamma_k' \leq \gamma_{k+1}$, 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 $\sigma_{\mathrm{ess}}(H_D) = \sigma_{\mathrm{ess}}(H)$ and $\sigma_{\mathrm{ess}}(H_{t,D}) = \sigma_{\mathrm{ess}}(H_t)$.

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 $\varphi_k(x) \coloneqq \varphi(x/k)$ 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 $\psi_k \coloneqq 1 - \varphi_k$. 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 $k \coloneqq n/4$, for $n \in \mathbb{N}$.

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

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

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

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

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

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

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 $\operatorname{dist}(\eta, \sigma(H_{n,0})) \ge \delta_0 > 0$ 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 $u_{n_j}^{(1)}, \dots, u_{n_j}^{(\ell)}$ 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

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

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.

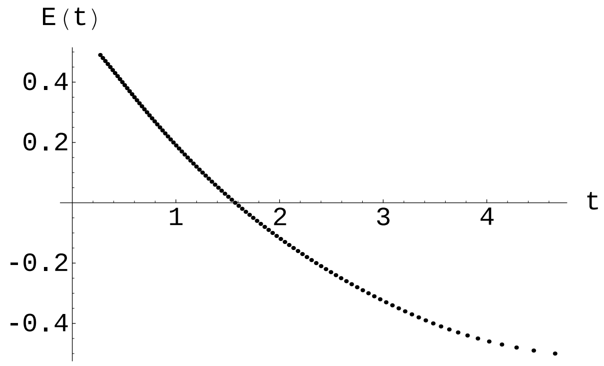

Figure 1.1: An eigenvalue branch of H_t in the first spectral gap.

1.6 Periodic potentials on the strip and the plane

Let $V : \mathbb{R}^2 \to \mathbb{R}$ be $\mathbb{Z}^2$-periodic and Lipschitz-continuous and let $\Sigma = \mathbb{R} \times (0,1)$ denote the infinite strip of width 1. We denote by S_t the (self-adjoint) operator $-\Delta + W_t$, acting in $L_2(\Sigma)$, with periodic boundary conditions in the y-variable and with W_t now defined as

$$W_t(x,y) := \begin{cases} V(x,y), & x \geq 0, \\ V(x+t,y), & x < 0, \end{cases} \qquad 0 \leq 1 \leq t. \tag{1.26}$$

Since S_0 is periodic in the x-variable, its spectrum has a band-gap structure.

We first observe that the essential spectrum of the family S_t does not depend on the parameter t, i.e., $\sigma_{\mathrm{ess}}(S_t) = \sigma_{\mathrm{ess}}(S_0)$ for all $t \in [0,1]$. As in Section 1.3, this follows from the compactness of $(S_t - c)^{-1} - (S_{t,D} - c)^{-1}$, where $S_{t,D}$ is S_t with an additional Dirichlet boundary condition at $x = 0$, say. (While, in one dimension, adding in a Dirichlet boundary condition at a single point causes a rank-one perturbation of the resolvent, the resolvent difference is now Hilbert-Schmidt, which can be seen from the following well-known line of argument: If $-\Delta_\Sigma$ denotes the (negative) Laplacian in $L_2(\Sigma)$ and $-\Delta_{\Sigma;D}$ is the (negative) Laplacian in $L_2(\Sigma)$ with an additional Dirichlet boundary condition at $x = 0$, then $(-\Delta_\Sigma + 1)^{-1} - (-\Delta_{\Sigma;D} + 1)^{-1}$ has an integral kernel which can be written down explicitly using the Green's function for $-\Delta_\Sigma$ and the reflection principle, cf. Exercise 6.

While the essential spectrum of the family S_t does not change as t ranges through $[0,1]$, S_t will have discrete eigenvalues in the spectral gaps of S_0 for appropriate values of t. We have the following result.

Theorem 1.16. *Let (a,b), $a < b$, denote a spectral gap of S_t and let $E \in (a,b)$. Then there exists $t = t_E \in (0,1)$ such that E is a discrete eigenvalue of S_t.*

Proof.

(1) As on the real line, we work with approximating problems on finite size sections of the infinite strip Σ. Let

$$\Sigma_{n,t} := (-n-t, n) \times (0,1), \quad n \in \mathbb{N}, \tag{1.27}$$

and consider $S_{n,t} := -\Delta + W_t$ acting in $L_2(\Sigma_{n,t})$ with periodic boundary conditions in both coordinates. The operator $S_{n,t}$ has compact resolvent and purely discrete spectrum accumulating only at $+\infty$. The rectangles $\Sigma_{n,0}$ (respectively, $\Sigma_{n,1}$) consist of $2n$ (respectively, $2n+1$) period cells. By routine arguments (see, e.g., [RS-IV, E]), the number of eigenvalues below the gap (a,b) is an integer multiple of the number of cells in these rectangles; we conclude, that eigenvalues of $S_{n,t}$ must cross the gap as t increases from 0 to 1.

(2) Let $E \in (a,b)$. According to (1), for any $n \in \mathbb{N}$ we can find $t_n \in (0,1)$ such that $E \in \sigma_{\mathrm{disc}}(S_{n,t_n})$; then there are eigenfunctions $u_n \in D(S_{n,t_n})$ with $S_{n,t_n} u_n = E u_n$, $\|u_n\| = 1$, and $\|\nabla u_n\| \leq C$ for some constant $C \geq 0$. We now choose cut-off functions φ_n as in Section 1.4 and denote the natural extension to $\mathbb{R}^2$ again by φ_n. We also let $\psi_n = 1 - \varphi_n$. Clearly,

$$\left\|(S_{t_n} - E)(\varphi_{n/4} u_n)\right\|, \ \left\|(S_{n,t_n} - E)(\psi_{n/4} u_n)\right\| \leq c/n, \tag{1.28}$$

for some $c \geq 0$. There is a subsequence $(t_{n_j})_{j\in\mathbb{N}} \subset (t_n)_{n\in\mathbb{N}}$ and $\bar{t} \in [0,1]$ s.th. $t_{n_j} \to \bar{t}$ as $j \to \infty$. Since V is Lipschitz, we may infer from (1.28) that

$$\left\|(S_{\bar{t}} - E)(\varphi_{n_j/4} u_{n_j})\right\| \to 0, \qquad j \to \infty, \tag{1.29}$$

and it remains to show that $\left\|\psi_{n/4} u_n\right\| \to 0$ so that $\left\|\varphi_{n/4} u_n\right\| \to 1$. We associate with functions $v\colon \Sigma_{n,t} \to \mathbb{C}$ functions $\tilde{v}\colon \Sigma_{n,0} \to \mathbb{C}$ by

$$\tilde{v}(x,y) := \begin{cases} v(x,y), & x > 0, \\ v(x-t,y), & x < 0, \end{cases} \tag{1.30}$$

in analogy with (1.15). Then $[\psi_{n/4} u_n]^\sim \in D(S_{n,0})$ and

$$\left\|(S_{n,0} - E)[\psi_{n/4} u_n]^\sim\right\| = \left\|(S_{n,t_n} - E)(\psi_{n/4} u_n)\right\| \leq c/n. \tag{1.31}$$

Since $(a,b) \cap \sigma(S_{n,0}) = \emptyset$ for all $n \in \mathbb{N}$, and since $E \in (a,b)$, the Spectral Theorem implies that $[\psi_{n/4} u_n]^\sim \to 0$ (and therefore also $\psi_{n/4} u_n \to 0$) as $n \to \infty$.

We therefore have shown that the functions $v_{n_j} := \varphi_{n_j/4} u_{n_j}$ for $j \in \mathbb{N}$ satisfy $\left\|(S_{\bar{t}} - E) v_{n_j}\right\| \to 0$ and $\left\|v_{n_j}\right\| \to 1$ as $j \to \infty$ which implies $E \in \sigma(S_{\bar{t}})$. □

Remark 1.17. By a well-known line of argument, one can obtain *exponential localization* of the eigenfunctions of S_t near the interface $\{(x,y) \mid x = 0\}$. Suppose that $E \in (a,b)$ and $t \in (0,1)$ satisfy $E \in \sigma(S_t)$. Let $u \in D(S_0) = D(S_t)$ denote a normalized eigenfunction and let φ_n, $n \in \mathbb{N}$, be as in the proof of Theorem 1.16. As above, we have

$$r_n := (S_t - E)(\varphi_n u) = -2\nabla\varphi_n \cdot \nabla u - (\Delta\varphi_n)u, \tag{1.32}$$

where $\|r_n\| \leq c/n$, for $n \in \mathbb{N}$. Since r_n has support in the interval $(-2n-1, 2n)$ we now see that there exist constants $C \geq 0$ and $\alpha > 0$ such that

$$\left\|\chi_{|x|\geq 4n} u\right\| \leq \left\|\chi_{|x|\geq 4n}(S_t - E)^{-1} r_n\right\| \leq C\mathrm{e}^{-\alpha n}, \tag{1.33}$$

by standard exponential decay estimates for the resolvent kernel of Schrödinger operators, cf., e.g., [S].

We now turn to the dislocation problem on the plane $\mathbb{R}^2$ where we study the operators

$$D_t = -\Delta + W_t, \quad 0 \leq t \leq 1. \tag{1.34}$$

Denote by $S_t(\vartheta)$ the operator S_t with ϑ-periodic boundary conditions in the y-variable. Since W_t is periodic with respect to y, we have

$$D_t \simeq \int_{[0,2\pi]}^{\oplus} S_t(\vartheta)\frac{\mathrm{d}\vartheta}{2\pi}, \tag{1.35}$$

and hence the spectrum of D_t has a band-gap structure; furthermore, D_t has no singular continuous part. As for the spectrum of S_t inside the gaps of S_0, Theorem 1.16 leads to the following result.

Theorem 1.18. *Let (a, b) denote a spectral gap of D_0, $a > \inf \sigma_{\mathrm{ess}}(D_0)$, and let $E \in (a, b)$. Then there exists $t = t_E \in (0, 1)$ with $E \in \sigma(D_t)$.*

Proof. Let $\varphi_n u_n \in D(S_t)$ as in part (2) of the proof of Theorem 1.16 denote an approximate solution of the eigenvalue problem for S_t and E. We extend u_n to a function $\tilde{u}_n(x, y)$ on $\mathbb{R}^2$ which is periodic in y. Writing $\Phi_n = \Phi_n(x, y) := \varphi_n(x)\varphi_n(y)$ we compute

$$\begin{aligned}(D_t - E)(\Phi_n \tilde{u}_n) &= \left(-\partial_x^2 - \partial_y^2 + W_t - E\right)(\varphi_n(x)\varphi_n(y)\tilde{u}_n(x, y)) \\ &= \varphi_n(y)[(S_t - E)(\varphi_n(x)u_n)]^{\sim} - \varphi_n(x)\left(2\varphi_n'(y)\partial_y\tilde{u}_n + \varphi_n''(y)\tilde{u}_n\right).\end{aligned} \tag{1.36}$$

The norms of the three terms on the RHS can be estimated (up to a constant which is independent of n) by εn, $\frac{1}{n}n$ and $\frac{1}{n^2}n$, respectively, and we see that

$$\|(D_t - E)(\Phi_n \tilde{u}_n)\| \leq c_0(1 + n\varepsilon), \tag{1.37}$$

while $\|\Phi_n \tilde{u}_n\| \geq c_0 n$ with a constant $c_0 > 0$. This implies the desired result. □

Remark 1.19. We learn from the above proof that there are functions

$$v_n = v_n(x,y) := \frac{1}{\|\Phi_n \tilde{u}_n\|}\Phi_n \tilde{u}_n \tag{1.38}$$

that satisfy $\|v_n\| = 1$, supp $v_n \subset [-n,n]^2$ and

$$(D_t - E)v_n \to 0, \qquad n \to \infty. \tag{1.39}$$

These functions will play a key role in our analysis of the rotation problem at small angle henceforth.

1.7 Density of states

We finally turn to a brief discussion of the i.d.s. (the integrated density of states) for the dislocation operators D_t. One distinguishes between *bulk* and *surface* states: Roughly speaking, the bulk states correspond to states away from the interface with energies in the spectral bands while the surface states for $0 < t < 1$ are produced by the interface and are (exponentially) localized near the interface. The (integrated) density of states measures for the bulk and surface states use a different scaling factor in the following definition: restricting D_t to large squares $Q_n = (-n,n)^2$ and taking Dirichlet boundary conditions, we obtain the operators $D_t^{(n)}$. For $I \subset \mathbb{R}$ an open interval, let $N(I, D_t^{(n)})$ denote the number of eigenvalues of $D_t^{(n)}$ in I, counting multiplicities. We then define for open intervals $I \subset \mathbb{R}$ and $J \subset \mathbb{R} \setminus \sigma(D_0)$ with $\overline{J} \subset \mathbb{R} \setminus \sigma(D_0)$

$$\rho_{\text{bulk}}(I, D_t) = \lim_{n\to\infty} \frac{1}{4n^2} N(I, D_t^{(n)}), \quad \rho_{\text{surf}}(J, D_t) = \lim_{n\to\infty} \frac{1}{2n} N(J, D_t^{(n)}). \tag{1.40}$$

The existence of the limits in (1.40) has been established in [EKSchrS, KS] for ergodic Schrödinger operators. Note that the surface density of states measure is defined (and possibly non-zero) for subintervals of the spectral bands, but then (1.40) is not suited to capture the surface states (cf. [EKSchrS, KS]).

The fact that the surface density of states exists does not mean it is non-zero and there are only rare examples where we know ρ_{surf} to be non-trivial. It is one of the main results of the present paper to show that dislocation moves enough states through the gap to have a non-trivial surface density of states, for suitable parameters t. Indeed, it is now easy to derive the following result:

Corollary 1.20. *Let (a,b) be a spectral gap of D_0 with $a > \inf \sigma_{\text{ess}}(D_0)$, and let $\emptyset \neq J \subset (a,b)$ be an open interval. Then there is a $t \in (0,1)$ such that $\rho_{\text{surf}}(J, D_t) > 0$.*

Proof. Let $[\alpha, \beta] \subset J$ with $\alpha < \beta$, fix $E \in (\alpha, \beta)$, and let $0 < \varepsilon < \min\{E-\alpha, \beta-E\}$. By Theorem 1.18 and Remark 1.19 there exist $t = t_E \in (0,1)$ and a function u_0

in the domain of D_t satisfying $\|u_0\| = 1$, supp u_0 compact, and $\|(D_t - E)u_0\| < \varepsilon$. Let $\nu \in \mathbb{N}$ be such that supp $u_0 \subset (-\nu, \nu)^2$; note that, in the present proof, ν corresponds to the n of Remark 1.19. We then see that the functions φ_k, defined by $\varphi_k(x, y) := u_0(x, y - 2k\nu)$ for $k \in \mathbb{N}$, have pairwise disjoint supports, are of norm 1, and satisfy $\|(D_t - E)\varphi_k\| < \varepsilon$. Furthermore, we have supp $\varphi_k \subset (-n, n)^2$ provided $(2k+1)\nu < n$. Denoting $\mathcal{M}_n := \operatorname{span}\{\varphi_k;\, k \in \mathbb{N},\, k \le \frac{1}{2}(\frac{n}{\nu} - 1)\}$, it is clear that $\dim \mathcal{M}_n \ge n/(3\nu)$, for all n large. Let $\mathcal{N}_n$ denote the range of the spectral projection $P_{(\alpha,\beta)}(D_t^{(n)})$ of $D_t^{(n)}$ associated with the interval (α, β); we will show that $\dim \mathcal{N}_n \ge \dim \mathcal{M}_n$ which implies the desired result. If we assume for a contradiction that $\dim \mathcal{N}_n < \dim \mathcal{M}_n$ for some $n \in \mathbb{N}$, we can find a function $v \in \mathcal{M}_n \cap \mathcal{N}_n^{\perp}$ of norm 1. By the Spectral Theorem, $\|(D_t^{(n)} - E)v\| \ge \varepsilon$. On the other hand, v is a finite linear combination of the φ_k, which implies $\|(D_t^{(n)} - E)v\| < \varepsilon$. $\square$

We will continue the discussion of bulk versus surface states in the next chapter where a corresponding upper bound of the form $N(J, D_t^{(n)}) \le cn \log n$ is provided.

1.8 Muffin tin potentials

Here we present some simple examples where one can see the behavior of surface states directly. We will deal with $\mathbb{Z}^2$-periodic muffin tin potentials of infinite height (or depth) on the plane $\mathbb{R}^2$ which can be specified by fixing a radius $0 < r < 1/2$ for the discs where the potential vanishes, and the center $P_0 = (x_0, y_0) \in [0, 1)^2$ for the generic disc. In other words, we consider the periodic sets

$$\Omega_{r,P_0} := \cup_{(i,j)\in\mathbb{Z}^2} B_r(P_0 + (i, j)),$$

and we let $V = V_{r,P_0}$ be zero on Ω_{r,P_0} while we assume that V is infinite on $\mathbb{R}^2 \setminus \Omega_{r,P_0}$. If H_{ij} is the Dirichlet Laplacian of the disc $B_r(P_0 + (i, j))$, then the form-sum of $-\Delta$ and V_{r,P_0} is $\oplus_{(i,j)\in\mathbb{Z}^2} H_{ij}$. Without loss of generality, we may assume $y_0 = 0$ henceforth.

(1) Dislocation in the x-direction. Here muffin tin potentials yield an illustration for some of the phenomena encountered in Section 1.7. In the simplest case we would take $x_0 = 1/2$ so that the disks $B_r(1/2 + i, j)$, for $i \in \mathbb{N}_0$ and $j \in \mathbb{Z}$, will not intersect or touch the interface $\{(x, y);\, x = 0\}$. Defining the dislocation potential W_t as in (1.26), we see that there are bulk states given by the Dirichlet eigenvalues of all the discs that do not meet the interface, and there may be surface states given as the Dirichlet eigenvalues of the sets $B_r(1/2 - t, j) \cap \{x < 0\}$ for $j \in \mathbb{Z}$ and $1/2 - r < t < 1/2 + r$.

More precisely, let $\mu_k = \mu_k(r)$ denote the Dirichlet eigenvalues of the Laplacian on the disc of radius r, ordered by min-max and repeated according to their respective multiplicities. The Dirichlet eigenvalues of the domains $B_r(1/2 - t, 0) \cap \{x < 0\}$,

$1/2 - r < t < 1/2 + r$, are denoted as $\lambda_k(t) = \lambda_k(t, r)$; they are continuous, monotonically decreasing functions of t and converge to μ_k as $t \uparrow 1/2 + r$ and to $+\infty$ as $t \downarrow 1/2 - r$. In this simple model, the eigenvalues μ_k correspond to the bands of a periodic operator. We see that the gaps are crossed by surface states as t increases from 0 to 1, in accordance with the results of Section 1.7 (Corollary 1.20).

Along the same lines, one can easily analyze examples where x_0 is different from $1/2$; here more complicated geometric shapes may come into play.

(2) Dislocation in the y-direction. This problem has not been considered so far. We include a brief discussion of this case for two reasons: on the one side, we observe a new phenomenon which did not appear so far; on the other hand, one can see from our example that, presumably, there is no general theorem for translation of the left half-plane in the y-direction.

Let $V = V_r$ denote the muffin tin potential defined above, with $x_0 = y_0 = 0$. We then let $\tilde{W}_t$ coincide with V in the right half-plane, while we take $\tilde{W}_t(x, y) = V(x, y - t)$ in the left half-plane. At the interface $\{x = 0\}$ we see half-discs on the left and on the right with the half-discs on the right being fixed while the half-discs on the left are shifted by t in the y-direction. The surface states correspond to the states of the Dirichlet Laplacian on the union $\Omega_{t,r;\mathrm{surf}}$ of these half-discs. There are two cases: either $\Omega_{t,r;\mathrm{surf}}$ is connected and we have a scattering channel along the interface, or $\Omega_{t,r;\mathrm{surf}}$ is the disjoint union of a sequence of bounded domains; cf. Figure 1.2. In the second case, the eigenvalues on such domains start at the Dirichlet eigenvalues of the disc of radius r, increase up to the corresponding eigenvalues of a half-disc, and then move down again to where they started. For $1/4 < r < 1/2$, the picture is more complicated: If we let $\tau_0 = 1 - 2r$, $\tau_1 = 2r$, we find that the sets $\Omega_{t,r;\mathrm{surf}}$ are disconnected for $0 \leq t \leq \tau_0$ and for $\tau_1 \leq t \leq 1$; for $\tau_0 < t < \tau_1$, however, $\Omega_{t,r;\mathrm{surf}}$ is connected and forms a periodic wave guide with purely a.c. spectrum. We therefore observe a dramatic change in the spectrum of the dislocation operators: for $t \in [0, \tau_0] \cup [\tau_1, 1]$ the surface states in the gap are given by eigenvalues of infinite multiplicity while for $t \in (\tau_0, \tau_1)$ the surface states form bands of a.c. spectrum in the gaps. Note that, if we had chosen $x_0 = 1/2$, then nothing at all would have happened for translation in the y-direction.

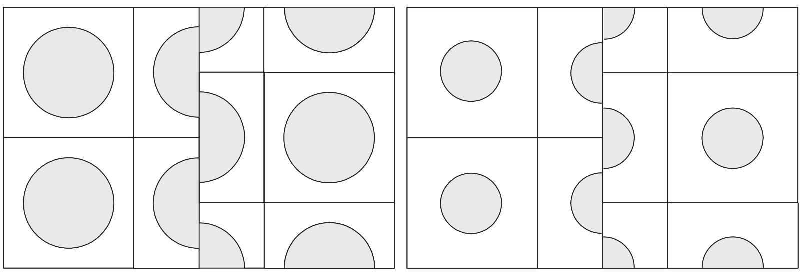

Figure 1.2: Muffin tins: two cases for dislocation in the y-direction.

Chapter 2

The rotation problem

2.1 Introduction

In this lecture we are interested in quantum mechanical models for solid states referring to situations where periodicity holds only in subsets of the sample; more precisely, the sample is the disjoint union of subsets such that, in each subset, the potential is obtained by restricting different periodic potentials to the corresponding subsets. Such zones or "grains" occur frequently in crystals and in alloys; some typical examples are shown in Figure 2.1. It is an important issue to understand how the interface between two grains will influence the energy spectrum of the sample. Typically, the grain boundaries appear to be (piecewise) linear, and one is led to study problems on $\mathbb{R}^2$ with a potential $W = W(x, y)$ defined by

$$W(x,y) := \begin{cases} V_r(x,y), & x \geq 0, \\ V_\ell(x,y), & x < 0, \end{cases} \tag{2.1}$$

where $V_r, V_\ell \colon \mathbb{R}^2 \to \mathbb{R}$ are periodic. While in the last chapter, V_ℓ is obtained from V_r by a translation, we now focus on models with a rotation about the origin. We will use some results on the translational problem to obtain spectral information about rotational problems in the limit of small angles. Our main theorem deals with the following situation. Let $V \colon \mathbb{R}^2 \to \mathbb{R}$ be a Lipschitz-continuous function which is periodic w.r.t. the lattice $\mathbb{Z}^2$. For $\vartheta \in (0, \pi/2)$, let

$$M_\vartheta := \begin{pmatrix} \cos\vartheta & -\sin\vartheta \\ \sin\vartheta & \cos\vartheta \end{pmatrix} \in \mathbb{R}^{2\times 2}, \tag{2.2}$$

and

$$V_\vartheta(x,y) := \begin{cases} V(x,y), & x \geq 0, \\ V(M_{-\vartheta}(x,y)), & x < 0. \end{cases} \tag{2.3}$$

We then let H_0 denote the (unique) self-adjoint extension of $-\Delta \restriction C_c^\infty(\mathbb{R}^2)$, acting in the Hilbert space $L_2(\mathbb{R}^2)$, and

$$R_\vartheta := H_0 + V_\vartheta, \qquad D(R_\vartheta) = D(H_0). \tag{2.4}$$

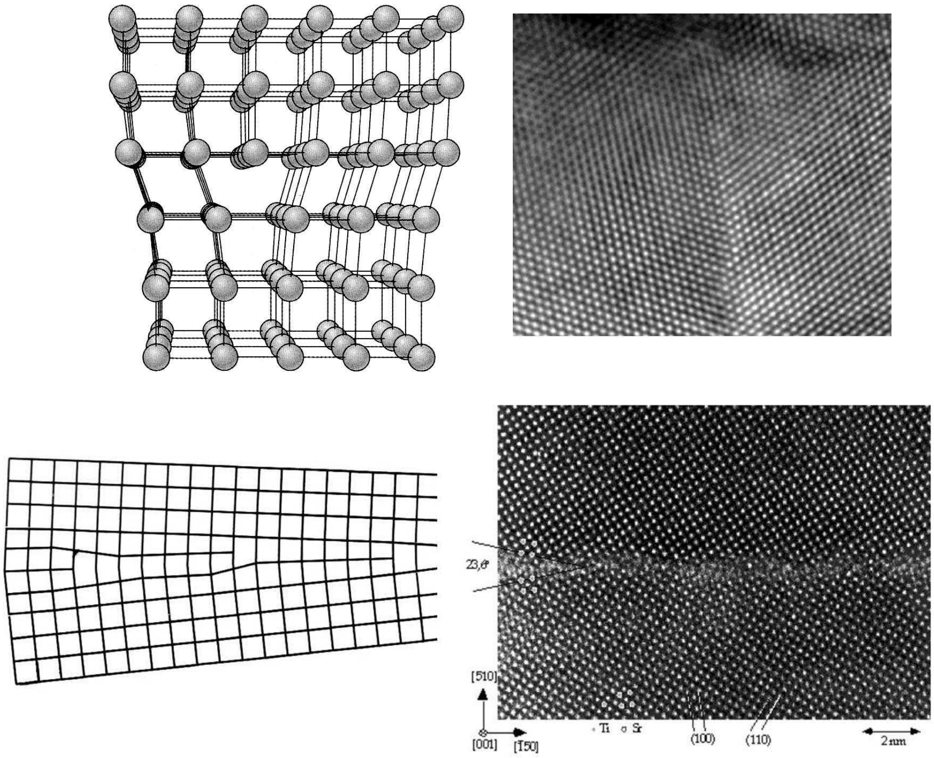

Figure 2.1: Edge dislocation and small angle grain boundary.

Then R_ϑ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^2)$ and semi-bounded from below. Our main assumption is that the periodic Hamiltonian $H := H_0 + V = R_0$ has a gap (a, b) in the essential spectrum $\sigma_{\mathrm{ess}}(H)$, i.e., we assume that there exist $a < b \in \mathbb{R}$ that satisfy $\inf \sigma_{\mathrm{ess}}(H) < a$ and $(a, b) \cap \sigma(H) = \emptyset$; we do not need to assume that a, b are the actual gap edges. It is easy to see (using, e.g., [RS-I; Thm. VIII.25]) that the operators R_ϑ converge to R_{ϑ_0} in the strong resolvent sense as $\vartheta \to \vartheta_0 \in [0, \pi/2)$; in particular, R_ϑ converges to H in the strong resolvent sense as $\vartheta \to 0$. Recall that strong resolvent convergence implies upper semi-continuity of the spectrum while the spectrum may contract considerably when the limit is reached. Here we are dealing with a situation where the spectrum in fact behaves discontinuously at $\vartheta = 0$ since, counter to first intuition, the spectrum of R_ϑ "fills" the gap (a, b) as $\vartheta \to 0$ with $\vartheta > 0$. This implies, in particular, that R_ϑ cannot converge to H in the norm resolvent sense, as $\vartheta \to 0$.

Theorem 2.1. *Let H, R_ϑ and (a, b) as above. Then, for any $\varepsilon > 0$ there exists $0 < \vartheta_\varepsilon < \pi/2$ such that for any $E \in (a, b)$ we have*

$$\sigma(R_\vartheta) \cap (E - \varepsilon, E + \varepsilon) \neq \emptyset, \qquad \forall 0 < \vartheta < \vartheta_\varepsilon. \tag{2.5}$$

Remark 2.2.

(i) Roughly speaking, the moment we start rotating the potential on the left-hand side by a tiny angle the gap (a, b) is suddenly full of spectrum of R_ϑ in the sense that, for $0 < \vartheta < \vartheta_\varepsilon$, no gap of R_ϑ in the interval (a, b) can have length larger than 2ε. It is conceivable that for most ϑ the spectrum of R_ϑ covers the interval (a, b), but we will see that there are examples where R_ϑ has gaps in (a, b) for some ϑ.

(ii) It seems to be quite hard to determine the nature of the spectrum of R_ϑ for general $\vartheta \in (0, \pi/2)$; however, we will point out that there are some special angles for which singular continuous spectrum can be excluded.

(iii) In addition to what is stated in Theorem 2.1 it is our goal to obtain lower and upper bounds for the spectral densities in the intervals $(E - \varepsilon, E + \varepsilon)$ on a scale that is appropriate to surface states (without knowing that an integrated surface density of states exists for R_ϑ).

There is a simple, intuitive connection between the rotational problem and the related translational problem, given as follows: Starting from the same periodic potential V as above, we again consider the potential W_t in (1.26) given by

$$W_t(x, y) := \begin{cases} V(x, y), & x \geq 0, \\ V(x + t, y), & x < 0, \end{cases} \qquad 0 \leq 1 \leq t,$$

and define $D_t := -\Delta + W_t$, acting in $L_2(\mathbb{R}^2)$. In Chapter 3.2 we have seen that spectrum of D_t crosses the gap as t varies between 0 and 1. Now our key observation consists in the following: for any given $\varepsilon > 0$ and $n \in \mathbb{N}$, we can find points $(0, \eta)$ on the y-axis such that

$$|V_\vartheta(x, y) - W_t(x, y)| < \varepsilon, \qquad (x, y) \in Q_n(0, \eta), \tag{2.6}$$

with $Q_n(0, \eta) = (-n, n) \times (\eta - n, \eta + n)$, provided $\vartheta > 0$ is small enough and satisfies a condition which ensures an appropriate alignment of the period cells on the y-axis. First of all, we recapitulate some results concerning the dislocation problem on the plane.

2.2 The dislocation problem on a strip and for the plane

Let $V : \mathbb{R}^2 \to \mathbb{R}$ be $\mathbb{Z}^2$-periodic and Lipschitz-continuous, let $I := (0, 1)$, and let $\Sigma := \mathbb{R} \times (0, 1) = \mathbb{R} \times I$ denote the infinite strip of width 1. As before, we write $H := -\Delta + V$ for the (self-adjoint) Schrödinger operator with potential V acting in

$L_2(\mathbb{R}^2)$. Then $\sigma(H)$, the spectrum of H, has band structure, i.e., it is the (locally finite) union of compact intervals [RS-IV]. The intervals of spectrum, the *bands*, may be separated by (open) intervals, the *gaps*. Moreover, $\sigma(H)$ is purely absolutely continuous. For $0 \le t \le 1$, we introduce the self-adjoint operators

$$\begin{aligned} S_t &:= -\Delta + W_t, \quad \text{acting in } L_2(\Sigma), \\ D_t &:= -\Delta + W_t, \quad \text{acting in } L_2(\mathbb{R}^2), \end{aligned} \tag{2.7}$$

where S_t has periodic boundary conditions in the y-variable and W_t is as in (1.26). Since V is bounded, the domains $D(\cdot)$ of the above operators satisfy $D(D_t) = D(H)$ and $D(S_t) = D(H_{0,\Sigma})$, for all t, where $H_{0,\Sigma}$ denotes the Laplacian on Σ with periodic boundary conditions in y. The operator $-\Delta+W_t$ in $L_2(\Sigma)$ with ϑ-periodic boundary conditions in y is denoted by $S_t(\vartheta)$, for $0 \le \vartheta \le 2\pi$. As usual, D_t can be obtained from the $S_t(\vartheta)$ as a direct fiber integral,

$$D_t = \int_{0\le\vartheta\le 2\pi}^{\oplus} S_t(\vartheta)\frac{d\vartheta}{2\pi}; \tag{2.8}$$

direct fiber integrals are discussed, e.g., in [RS-IV]; see also Exercise 7. As a consequence, for any ϑ the spectrum of $S_t(\vartheta)$ is a subset of $\sigma(D_t)$. Furthermore, using the periodicity in the x-direction, each $S_t(\vartheta)$ can itself be written as a direct fiber integral and so the spectrum of $S_t(\vartheta)$ is purely essential spectrum with a band-gap structure.

Proposition 2.3. *Let (a, b) denote a spectral gap of H and let $E \in (a, b)$. Then there exists some $t = t_E \in (0, 1)$ such that E is a (discrete) eigenvalue of S_{t_E}.*

Moreover, for any $n \in \mathbb{N}$ there are functions $v_n = v_n(x, y)$ in the domain of S_t that satisfy $\|v_n\| = 1$, supp $v_n \subset [-n, n] \times [0, 1]$ *and $(S_{t_E} - E)v_n \to 0$ as $n \to \infty$.*

The functions v_n constructed above satisfy periodic boundary conditions with respect to y and may thus be extended to y-periodic functions $\tilde{v}_n$ on $\mathbb{R}^2$. Applying also cut-offs $\psi_n = \varphi_n(y)$ in the y-direction, we let

$$w_n := \frac{1}{\|\psi_n \tilde{v}_n\|}\psi_n \tilde{v}_n; \tag{2.9}$$

the w_n satisfy $\|w_n\| = 1$, $w_n \in D_{t_n}$ and $(D_{t_n} - E)w_n \to 0$ as $n \to \infty$. By the same argument as above this leads to $E \in \sigma(D_{t_E})$ (where, again $t_E = \lim t_n$) and we have thus obtained:

Proposition 2.4. *Let (a, b) denote a spectral gap of H and let $E \in (a, b)$. Then there exists $t = t_E \in (0, 1)$ such that $E \in \sigma(D_{t_E})$.*

Moreover, for any $n \in \mathbb{N}$ there are functions $w_n = w_n(x, y)$ in the domain of D_t that satisfy $\|w_n\| = 1$, supp $w_n \subset [-n, n]^2$ *and $(D_{t_E} - E)w_n \to 0$ as $n \to \infty$.*

Note that the spectrum of D_t inside (a, b) will again consist of bands which we could find by repeating the above process for all ϑ-periodic boundary conditions w.r.t. y.

2.3 The rotation problem for small angles

In this section, we study the spectrum of the operators R_ϑ, for $0 < \vartheta < \pi/2$, where the R_ϑ are defined in (2.4) as self-adjoint operators in the Hilbert space $L_2(\mathbb{R}^2)$.

In view of a proof of Theorem 2.1, consider a fixed $E \in (a, b)$. Then, by Proposition 2.4, there is some $t \in (0, 1)$ such that E is in the spectrum of the dislocation operator D_t on the plane. We wish to find angles ϑ with the property that the potential V_ϑ is approximately equal to W_t on a sufficiently large square $Q_n(0, \eta)$ of side-length $2n$, centered at some point $(0, \eta)$ on the y-axis. This leads to the following requirements: If we imagine the grid $\Gamma = \{(x, y) \in \mathbb{R}^2\,;\, x \in \mathbb{Z} \text{ or } y \in \mathbb{Z}\}$ of lines describing the period cells, we have to make sure that, inside $Q_n(0, \eta)$, the alignment between the horizontal lines of Γ in the right half-plane with the rotated horizontal lines of $M_\vartheta\Gamma$ in the left half-plane is nearly perfect on the y-axis and that the rotated vertical lines of $M_\vartheta\Gamma$ in the left half-plane have, roughly, distance t (modulo $\mathbb{Z}$) from the y-axis. More precisely, we wish to find $m \in \mathbb{N}$ such that $m/\cos\vartheta$ is integer, up to a small error, and $m \tan\vartheta = t\,(\mathrm{mod}\ \mathbb{Z})$, again up to a small error, inside $Q_n(0, \eta)$.

We first prepare a lemma which deals with ergodicity on the flat torus $\mathbb{T}^2 = \mathbb{R}^2/\mathbb{Z}^2$, as in [RS-I]. We consider transformations $T_\vartheta \colon \mathbb{T}^2 \to \mathbb{T}^2$ defined by

$$T_\vartheta(x, y) \coloneqq (x + \tan\vartheta, y + 1/\cos\vartheta). \tag{2.10}$$

Lemma 2.5. *There is a set $\Theta \subset (0, \pi/2)$ with countable complement such that the transformation T_ϑ in* (2.10) *is ergodic for all $\vartheta \in \Theta$.*

Proof. Exercise 8. □

Let us write $x_\sim$ for the fractional part of $x > 0$, i.e., $x_\sim = x - \lfloor x \rfloor$ if $x > 0$. In the proof of our main theorem, we will need natural numbers m such that, for $t \in (0, 1)$ given, $(m \tan\vartheta)_\sim$ is approximately equal to t and $(m/\cos\vartheta)_\sim$ almost equals 0. The existence of such numbers m follows from Lemma 2.5 and Birkhoff's Ergodic Theorem. Let $\vartheta \in \Theta$, $\varepsilon > 0$, and let us denote by χ_Q the characteristic function of the set $Q \coloneqq (t - \varepsilon, t + \varepsilon) \times (-\varepsilon, \varepsilon) \subset \mathbb{T}^2$. Then, for all $(x, y) \in \mathbb{T}^2$,

$$\lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} \chi_Q(T_\vartheta^m(x, y)) = \int_Q \mathrm{d}x\,\mathrm{d}y = 4\varepsilon^2 > 0, \tag{2.11}$$

and we may take $(x, y) \coloneqq (0, 0)$ to arrive at the desired result.

We add the following remarks to the above argument:

(1) Translation on the torus is a particularly simple ergodic transformation: for ϑ given, it can equivalently be seen as linear motion on parallel lines in $\mathbb{R}^2$, factored by $\mathbb{Z}^2$. In particular, two nearby points (x, y) and (x', y') will forever keep their relative position under the action of T_ϑ^m, and thus the statement of Birkhoff's Theorem holds for *any* point (x, y), not just for a.e. (x, y).

(2) In some sense, the Birkhoff Theorem is the strongest result one can use in this context. Similar results are obtained from Dirichlet's Theorem on the approximation of irrational numbers by rationals.

We are now ready for a first main result which establishes the existence of surface states in the gaps of H and shows that, in fact, any gap (a, b) of H is filling up with spectrum of R_ϑ as $\vartheta \to 0$.

Proposition 2.6. *Let (a, b) be a spectral gap of H and let $[\alpha, \beta] \subset (a, b)$, $\alpha < \beta$. Then there is a $\vartheta_0 = \vartheta_0(\alpha, \beta) > 0$ such that*

$$\sigma(R_\vartheta) \cap (\alpha, \beta) \neq \emptyset, \qquad \forall \vartheta \in (0, \vartheta_0). \tag{2.12}$$

Proof.

(1) We first restrict our attention to $\vartheta \in \Theta$ with Θ as in Lemma 2.5. Let $E \in (\alpha, \beta)$ and $\varepsilon := \min\{E - \alpha, \beta - E\}/2$. By Proposition 2.4, we can find $n = n_\varepsilon \in \mathbb{N}$ and a function u_n of norm 1 in the domain of D_t with supp $u_n \subset [-n, n]^2$ such that $\|(D_t - E)u_n\| < \varepsilon$. Obviously $u_{n,k}(x, y) := u_n(x, y - k)$ satisfies the same estimate for any $k \in \mathbb{N}$. If we can show that, for appropriate $k \in \mathbb{N}$,

$$|V_\vartheta(x, y) - W_t(x, y)| < \varepsilon, \qquad (x, y) \in Q_n(0, k) \tag{2.13}$$

(recall the definition of $Q_n(0, k) = (-n, n) \times (k - n, k + n)$), we may conclude that

$$\|(R_\vartheta - E)u_{n,k}\| < 2\varepsilon; \tag{2.14}$$

but then the Spectral Theorem implies that R_ϑ has spectrum inside the interval $(E - 2\varepsilon, E + 2\varepsilon) \subset (\alpha, \beta)$.

For a proof of (2.13), we first observe that by the properties of V and the definitions of V_ϑ and W_t, we have the following estimate:

$$|V_\vartheta(x, y) - W_t(x, y)|^2 \leq \min_{j_1, j_2 \in \mathbb{Z}} L^2((X - j_1)^2 + (Y - j_2)^2), \quad \forall (x, y) \in \mathbb{R}^2, \tag{2.15}$$

with

$$X := x(\cos\vartheta - 1) - t + y \sin\vartheta, \qquad Y := -x \sin\vartheta + y(\cos\vartheta - 1) \tag{2.16}$$

and L the Lipschitz constant of V. Now for $\vartheta \in \Theta$ given, there is some $m = m_\vartheta \in \mathbb{N}$ such that

$$\left(\frac{m}{\cos\vartheta}\right)_\sim < \varepsilon/4, \qquad |(m \tan\vartheta)_\sim - t| < \varepsilon/4; \tag{2.17}$$

in particular, there is some $N \in \mathbb{N}$ s.th. $|m/\cos\vartheta - N| < \varepsilon/4$.

We may now apply the estimate (2.15) to the points $(x, y) \in Q_n(0, N)$ to find

$$|V_\vartheta(x, y) - W_t(x, y)|^2 \leq L^2\left((X - \lfloor m \tan\vartheta \rfloor)^2 + (Y + N - m)^2\right), \tag{2.18}$$

for all $(x, y) \in Q_n(0, N)$. Here

$$|X - \lfloor m \tan\vartheta \rfloor| \le n(1-\cos\vartheta) + n\vartheta + |m\tan\vartheta - \lfloor m\tan\vartheta\rfloor - t| \le 2n_\varepsilon\vartheta + |(m\tan\vartheta)_\sim - t| \tag{2.19}$$

and

$$|Y + N - m| \le 2n_\varepsilon\vartheta + |N - m/\cos\vartheta|. \tag{2.20}$$

We choose $\vartheta_0 > 0$ small enough to have $2n_\varepsilon\vartheta_0 < \varepsilon/4$ and (2.13) follows if we pick $k \coloneqq N$. We have thus shown that R_ϑ has spectrum in (α, β) for all $\vartheta \in \Theta \cap (0, \vartheta_0)$.

(2) In order to remove the restriction $\vartheta \in \Theta$ we note that with each $\vartheta \in \Theta$ there comes a positive number $\eta_\vartheta > 0$ such that

$$\|(R_\sigma - E)u_{n,k}\| < 3\varepsilon, \quad \forall \sigma \in (\vartheta - \eta_\vartheta, \vartheta + \eta_\vartheta), \tag{2.21}$$

since

$$\|(V_\sigma - V_\vartheta) \restriction \operatorname{supp} u_{n,k}\|_\infty \to 0, \quad \sigma \to \vartheta. \tag{2.22}$$

As the intervals $(\vartheta - \eta_\vartheta, \vartheta + \eta_\vartheta)$ with ϑ ranging between 0 and ϑ_0 cover the interval $(0, \vartheta_0)$, the desired result follows. □

Now it is easy to obtain Theorem 2.1 in the Introduction from Proposition 2.6:

Proof of Theorem 2.1 For $\varepsilon > 0$ given, we consider points $a = \gamma_0 < \gamma_1 < \gamma_2 < \ldots < \gamma_N = b$ such that $\gamma_j - \gamma_{j-1} < \varepsilon/2$, for $j = 1, \ldots, N$. For each of the intervals $I_j \coloneqq (\gamma_{j-1}, \gamma_j)$, $2 \le j \le N-1$, Proposition 2.6 yields a constant $\vartheta_j > 0$ with the property that R_ϑ has spectrum in the interval I_j for all $0 < \vartheta < \vartheta_j$. Then $\vartheta_0 \coloneqq \min_{2\le j\le N-1} \vartheta_j$ has the required properties. □

2.4 Integrated density of states bounds

It is clear that ergodicity gives us not just a single m as in (2.17), for $\vartheta \in \Theta$; in fact, (2.11) guarantees that suitable m will appear with a certain frequency. We will use this observation to obtain lower bounds for a quantity which, in the limit, would translate into a (positive) lower bound for the surface i.d.s. measure if we knew that the required limit exists. This will be complemented by a similar upper bound which is of the expected order, up to a logarithmic factor.

Let $R_\vartheta^{(n)}$ denote the operator $-\Delta + V_\vartheta$, acting in $L_2(Q_n)$ with Dirichlet boundary conditions, where $Q_n \coloneqq (-n, n)^2 \subset \mathbb{R}^2$. For any interval $I \subset \mathbb{R}$, we denote by $N_I(R_\vartheta^{(n)})$ the number of eigenvalues of $R_\vartheta^{(n)}$ in I, each eigenvalue being counted according to its multiplicity. The existence of a surface i.d.s. measure in the gap (a, b) would correspond to the existence of a finite limit $\lim_{n\to\infty} \frac{1}{n} N_I(R_\vartheta^{(n)})$, for any interval I with $\overline{I} \subset (a, b)$. Theorem 2.7 below provides lower bounds of the form

$$\liminf_{n\to\infty} \frac{1}{n} N_I(R_\vartheta^{(n)}) > 0, \tag{2.23}$$

for (non-degenerate) subintervals I and small $\vartheta \in \Theta$, while Theorem 2.9 will yield an upper bound

$$\limsup_{n\to\infty} \frac{1}{n\log n} N_I(R_\vartheta^{(n)}) < \infty. \tag{2.24}$$

We begin with a lower bound.

Theorem 2.7. *Let H, R_ϑ as above and suppose that (a,b) is a spectral gap of H. Let Θ as in Lemma 2.5.*

Then, for any $\varepsilon > 0$ there exists a $\vartheta_\varepsilon > 0$ such that (2.23) holds for all $\vartheta \in \Theta \cap (0, \vartheta_\varepsilon)$ and for any interval $I \subset (a,b)$ of length greater than ε.

Proof.

(1) Let $[\alpha,\beta] \subset (a,b)$, fix $E \in (\alpha,\beta)$, and let $0 < \varepsilon < \min\{E-\alpha, \beta-E\}$. Let u_0 in the domain of D_t with compact support satisfy $\|u_0\| = 1$ and $\|(D_t - E)u_0\| < \varepsilon$, as in Proposition 2.4. Let $\nu \in \mathbb{N}$ be such that supp $u_0 \subset Q_\nu = (-\nu,\nu)^2$; note that, in this proof, ν corresponds to the parameter n that has been used so far.

Let $\vartheta \in \Theta \cap (0, \pi/4]$ so that, in particular, $1/\sqrt{2} \le \cos\vartheta \le 1$. By ergodicity, there exists a constant $c_0 = c_0(\vartheta) > 0$ with the following properties: for $n \in \mathbb{N}$ large, there are at least $J_n := \lfloor c_0 n \rfloor$ natural numbers $m_1, \ldots, m_{J_n} \in (0, n/4)$ such that (2.17) holds for $m = m_s$, $s = 1, \ldots, J_n$, and such that

$$|m_s - m_r| \ge 2\nu, \qquad s \neq r, \quad 1 \le s, r \le J_n; \tag{2.25}$$

here J_n and $m_1, \ldots, m_{J_n}$ depend on n and ϑ. It follows that for each $j = 1, \ldots, J_n$ there is some $N_j \in \mathbb{N}$ such that $|m_s/\cos\vartheta - N_j| < \varepsilon/4$ and $|m_s \tan\vartheta - t|_\sim < \varepsilon/4$. We then see that the functions φ_j, defined by $\varphi_j(x,y) := u_0(x, y - N_j)$, are of norm 1 and have mutually disjoint supports contained in $(-n,n)^2$. Furthermore, for ϑ small enough, $0 < \vartheta < \vartheta_\varepsilon$, say, we can show (as in the proof of Proposition 2.6) that an estimate (2.13) holds on each square $(-\nu,\nu) \times (N_j - \nu, N_j + \nu)$. Thus (2.13) holds on the support of each φ_j and it follows that

$$\left\| (R_\vartheta^{(n)} - E)\varphi_j \right\| < \varepsilon, \qquad 0 < \vartheta < \vartheta_\varepsilon, \quad j = 1, \ldots, J_n. \tag{2.26}$$

Then $\mathcal{M} := \operatorname{span}\{\varphi_j\,;\, j = 1, \ldots, J_n\}$ has dimension J_n. Let $\mathcal{N}$ denote the range of the spectral projection $P_{(\alpha,\beta)}(R_\vartheta^{(n)})$ of $R_\vartheta^{(n)}$ associated with the interval (α,β) and assume for a contradiction that $\dim\mathcal{N} < J_n$. Then we can find a function $v \in \mathcal{M} \cap \mathcal{N}^\perp$ of norm 1. By the Spectral Theorem, $\left\|(R_\vartheta^{(n)} - E)v\right\| \ge \varepsilon$. On the other hand, (2.26) together with $v = \sum_{i=1}^N a_i \varphi_i$ implies $\left\|(R_\vartheta^{(n)} - E)v\right\| < \varepsilon$ because the φ_j have mutually disjoint supports.

We have therefore shown that for any interval $I = [\alpha,\beta]$ there exists some $\vartheta_0 > 0$ such that (2.23) holds for all $\vartheta \in \Theta \cap (0, \vartheta_0)$.

(2) Now let $\varepsilon > 0$. As in the proof of Theorem 2.1, we may cover the interval (a,b) by a finite number of subintervals of length ε; applying the result of part (1) we then obtain the desired statement. $\square$

Remark 2.8.

(1) It appears that the argument used at the end of the proof of Proposition 2.6 to remove the restriction $\vartheta \in \Theta$ does not work in the context of Theorem 2.7.

(2) It follows from the proof of Theorem 2.7 that $\sigma_{\mathrm{ess}}(R_\vartheta) \cap I \neq \emptyset$ for all $\vartheta \in \Theta \cap (0, \vartheta_\varepsilon)$ and for any interval $I \subset (a, b)$ of length greater than ε.

We now complement the lower estimate established in Theorem 2.7 by an upper bound which is of the expected order, up to a logarithmic factor. Note that we treat a situation which is far more general than the rotation or dislocation problems studied so far. In fact, we will allow for different potentials V_1 on the left and V_2 on the right which are only linked by the assumption that there is a common spectral gap; neither V_1 nor V_2 are required to be periodic. The proof uses technology which is fairly standard and based on exponential decay estimates for resolvents.

Theorem 2.9. *Let V_1, $V_2 \in L_\infty(\mathbb{R}^2, \mathbb{R})$ and suppose that the interval $(a, b) \subset \mathbb{R}$ does not intersect the spectra of the self-adjoint operators $H_k := -\Delta + V_k$, $k = 1, 2$, both acting in the Hilbert space $L_2(\mathbb{R}^2)$. Let*

$$W := \chi_{\{x<0\}} \cdot V_1 + \chi_{\{x\geq 0\}} \cdot V_2 \tag{2.27}$$

and define $H := -\Delta + W$, a self-adjoint operator in $L_2(\mathbb{R}^2)$. Finally, we let $H^{(n)}$ denote the self-adjoint operator $-\Delta + W$ acting in $L_2(Q_n)$ with Dirichlet boundary conditions. Then, for any interval $[a', b'] \subset (a, b)$, we have

$$\limsup_{n\to\infty} \frac{1}{n \log n} N_{[a',b']}(H^{(n)}) < \infty. \tag{2.28}$$

Proof.

(1) We write $N(n) := N_{[a',b']}(H^{(n)})$ and note that there is a constant $c_0 \geq 0$ such that

$$N(n) \leq c_0 n^2, \qquad n \in \mathbb{N}; \tag{2.29}$$

this follows by routine min-max arguments as in [RS-IV; Section XIII.15].

(2) Let us consider the (normalized) eigenfunctions $u_{i,n}$ of $H^{(n)}$ associated with the eigenvalues $E_{i,n} \in [a', b']$, for $i = 1, \ldots, N(n)$. The main idea of the proof is to show that the $u_{i,n}$ are concentrated near the boundary of Q_n or near the y-axis. To obtain the corresponding estimates, we introduce the sets

$$\Omega_j(n) := \Omega_j^-(n) \cup \Omega_j^+(n), \qquad j \in \{1, 2, 3, 4\}, \tag{2.30}$$

where $\Omega_j^-(n) := \left(-\frac{n}{2} + \frac{2j}{\alpha}\log n, -\frac{2j}{\alpha}\log n\right) \times \left(-\frac{n}{2} + \frac{2j}{\alpha}\log n, \frac{n}{2} - \frac{2j}{\alpha}\log n\right)$, and $\Omega_j^+(n) := -\Omega_j^-(n)$ is the mirror-image of $\Omega_j^-(n)$ with respect to the y-axis; the parameter $\alpha > 0$ will be chosen as in (2.31) below. Note that, for $\alpha > 0$ fixed, the sets $\Omega_1(n), \dots, \Omega_4(n)$ are non-empty for n large. We have the trivial inclusions $\Omega_{j+1}(n) \subset \Omega_j(n)$ for $j = 1, 2, 3$.

We will use the following exponential decay estimate for the resolvent of the operators H_k: There are constants $C \geq 0$, $\alpha > 0$ such that for any $E \in [a', b']$ and (measurable) sets $K_1, K_2 \subset \mathbb{R}^2$ we have (cf., e.g., [AADH; Prop. 2.4])

$$\left\| \chi_{K_1} \partial_j^p (H_k - E)^{-1} \chi_{K_2} \right\| \leq C \mathrm{e}^{-\alpha \operatorname{dist}(K_1, K_2)}, \quad j, p \in \{0, 1\}, \quad k \in \{1, 2\}; \tag{2.31}$$

here $\partial_1 = \partial_x$, $\partial_2 = \partial_y$. We also choose cut-off functions $\varphi_n, \psi_n \in C_c^\infty(\mathbb{R}^2; \mathbb{R})$ satisfying

$$\operatorname{supp} \varphi_n \subset \Omega_1(n), \quad \varphi_n \restriction \Omega_2(n) = 1, \quad \operatorname{supp} \psi_n \subset \Omega_3(n), \quad \psi_n \restriction \Omega_4(n) = 1, \tag{2.32}$$

and $|\nabla \varphi_n|, |\nabla \psi_n|, |\partial_{ij} \varphi_n|, |\partial_{ij} \psi_n| \leq c (\log n)^{-1}$ with some constant $c \geq 0$; here $\varphi_n = \varphi_{n,\ell} + \varphi_{n,r}$ with $\varphi_{n,\ell}$ and $\varphi_{n,r}$ being supported in $\Omega_1^-(n)$ and $\Omega_1^+(n)$, respectively. By a well-known argument we can now derive the desired localization property: by the Leibniz rule, we have for $i = 1, \dots, N(n)$

$$(H_1 - E_i)(\varphi_{n,\ell} u_{i,n}) = (H^{(n)} - E_i)(\varphi_{n,\ell} u_{i,n}) = -2 \nabla \varphi_{n,\ell} \cdot \nabla u_{i,n} - \Delta \varphi_{n,\ell} u_{i,n} \tag{2.33}$$

so that

$$\chi_{\Omega_3^-(n)} u_{i,n} = -\chi_{\Omega_3^-(n)} (H_1 - E_i)^{-1} \chi_{\operatorname{supp} \nabla \varphi_{n,\ell}} [2 \nabla \varphi_{n,\ell} \cdot \nabla u_{i,n} + \Delta \varphi_{n,\ell} u_{i,n}]. \tag{2.34}$$

Using that $\operatorname{dist}(\Omega_3(n), \operatorname{supp} \nabla \varphi_n) \geq 2\alpha^{-1} \log n$ and $|\nabla \varphi_n|, |\Delta \varphi_n| \leq c (\log n)^{-1}$, the estimate (2.31) implies that

$$\left\| \chi_{\Omega_3(n)} u_{i,n} \right\|, \ \left\| \chi_{\Omega_3(n)} \nabla u_{i,n} \right\| \leq C (n^2 \log n)^{-1}, \qquad i = 1, \dots, N(n). \tag{2.35}$$

We now define $v_{i,n} := (1 - \psi_n) u_{i,n}$ and let $\mathcal{M}_n := \operatorname{span}\{v_{i,n}; i = 1, \dots, N(n)\}$. We claim that

$$\dim \mathcal{M}_n = N(n), \qquad n \geq n_0, \tag{2.36}$$

for some $n_0 \in \mathbb{N}$. Let $H_{Q_n \setminus \Omega_4(n)}$ be the operator $-\Delta + W$ on $Q_n \setminus \Omega_4(n)$ with Dirichlet boundary conditions. The functions $v_{i,n} := (1 - \psi_n) u_{i,n}$ are approximate eigenfunctions of $H_{Q_n \setminus \Omega_4(n)}$: in fact, using (2.35), one easily checks that

$$\left\| (H_{Q_n \setminus \Omega_4(n)} - E_{i,n}) v_{i,n} \right\| \leq C (n^2 \log^2 n)^{-1} \tag{2.37}$$

and

$$\| v_{i,n} - u_{i,n} \| \leq C (n^2 \log n)^{-1}, \tag{2.38}$$

for $i = 1, \dots, N(n)$. Now (2.29) and (2.38) imply $\sum_{i=1}^{N(n)} \| u_{i,n} - v_{i,n} \|^2 < 1$ for n large and we obtain (2.36).

(3) We next show that there is $n_1 \geq n_0 \in \mathbb{N}$ such that

$$\left\langle H_{Q_n \setminus \Omega_4(n)} w, w \right\rangle < b \, \|w\|^2, \qquad w \in \mathcal{M}_n, \quad n \geq n_1. \tag{2.39}$$

For a proof, consider an arbitrary $w = \sum_{i=1}^{N(n)} \gamma_i v_{i,n} \in \mathcal{M}_n$ with $\|w\| = 1$. Here we first observe that the coefficients γ_i satisfy a bound $|\gamma_i| \leq 2$, for n large, since (writing $\gamma^2 := \sum_i |\gamma_i|^2$ and $\eta_n^2 := \sum_i \|v_{i,n} - u_{i,n}\|^2$)

$$1 = \|w\| \geq \| \sum_{i=1}^{N(n)} \gamma_i u_{i,n}\| - \sum_{i=1}^{N(n)} |\gamma_i| \cdot \|v_{i,n} - u_{i,n}\| \geq \gamma(1 - \eta_n), \tag{2.40}$$

where $\eta_n \to 0$ as $n \to \infty$ by (2.38). Using (2.38) and the fact that $\nabla\psi_n$ and $\Delta\psi_n$ have support in $\Omega_3(n) \setminus \Omega_4(n)$, it follows that for n large

$$\|w\|^2 = \sum_{i=1}^{N(n)} |\gamma_i|^2 + r, \quad \langle H_{Q_n\setminus\Omega_4(n)} w, w\rangle = \sum_{i=1}^{N(n)} E_i |\gamma_i|^2 + r', \tag{2.41}$$

where $r, r' \leq C(\log n)^{-2}$, so that

$$\langle H_{Q_n\setminus\Omega_4(n)} w, w\rangle \leq b' \|w\|^2 + r'', \tag{2.42}$$

with $r'' \leq C(\log n)^{-2}$, for n large, and we obtain (2.39).

(4) We conclude from (2.39) that $\mathcal{M}_n \subset P_{(-\infty,b)}(H_{Q_n\setminus\Omega_4(n)})$ and then (2.36) implies that $\dim P_{(-\infty,b)}(H_{Q_n\setminus\Omega_4(n)}) \geq \dim \mathcal{M}_n = N(n)$. On the other hand, min-max arguments yield an upper bound for $\dim P_{(-\infty,b)}(H_{Q_n\setminus\Omega_4(n)})$ of the form $cn\log n$, and we are done. $\square$

2.5 Muffin tin potentials

In this section, we recourse to muffin tin potentials where one can arrive at rather precise statements that illustrate some of the phenomena described before. We will only look at muffin tin potentials with walls of infinite height and discuss the effect of the "filling up" of the gaps at small angles of rotation.

We consider the lattice $\mathbb{Z}^2 \subset \mathbb{R}^2$ where we first introduce the Laplacian of a periodic muffin tin with infinitely high walls separating the wells: for $0 < r < 1/2$, we let $D_r := B_r(\frac{1}{2}, \frac{1}{2})$ denote the disc of radius r centered at the point $(\frac{1}{2}, \frac{1}{2}) \in \mathbb{R}^2$, and generate from D_r the periodic sets

$$\Omega_r := \cup_{(i,j)\in\mathbb{Z}^2}(D_r + (i,j)), \qquad 0 < r < 1/2. \tag{2.43}$$

The Dirichlet Laplacian H_r of Ω_r is the direct sum of a countable number of copies of the Dirichlet Laplacian on D_r; therefore, the spectrum of H_r consists in a sequence of positive eigenvalues $(\mu_k(r))_{k\in\mathbb{N}}$ with $\mu_k(r) \to \infty$ as $k \to \infty$; we may assume that $\mu_k(r) < \mu_{k+1}(r)$ for all $k \in \mathbb{N}$. The eigenvalues $\mu_k = \mu_k(r)$ of H_r have infinite multiplicity. The μ_k correspond to the bands of a periodic problem: in fact, defining $V_r \colon \mathbb{R}^2 \to \mathbb{R}$ by

$$V_r(x,y) := \begin{cases} 0, & (x,y) \in \Omega_r, \\ 1, & (x,y) \notin \Omega_r, \end{cases} \tag{2.44}$$

the periodic Schrödinger operators $H_{r,n} := H_0 + nV_r$ have purely a.c. spectrum with a band-gap structure. Furthermore, norm resolvent convergence $H_{r,n} \to H_r$ implies that the bands of $H_{r,n}$ converge to the eigenvalues μ_k of H_r. In the sequel, denote by (a, b) one of the gaps (μ_k, μ_{k+1}). We next look at the rotation problem where we define

$$\Omega_{r,\vartheta} := (\Omega_r \cap \{x \geq 0\}) \cup ((M_\vartheta \Omega_r) \cap \{x < 0\})\,; \tag{2.45}$$

we also let $H_{r,\vartheta}$ denote the Dirichlet Laplacian on $\Omega_{r,\vartheta}$, for $0 < r < 1/2$ and $0 \leq \vartheta \leq \pi/4$.

The set $(M_\vartheta \Omega_r) \cap \{x < 0\}$ comes with two types of connected components: most (or, in some cases, all) components are discs, but typically there are also discs in $M_\vartheta \Omega_r$ with center at a distance less than r from the y-axis; those appear in $(M_\vartheta \Omega_r) \cap \{x < 0\}$ in a truncated form. It is then clear that $H_{r,\vartheta}$ has pure point spectrum.

Let us comment on some special cases before we proceed: for $\tan\vartheta$ rational, these truncated discs form a periodic pattern; furthermore, we will find a half-disc in $(M_\vartheta \Omega_r) \cap \{x < 0\}$ if and only if there is a disc in $M_\vartheta \Omega_r$ with center on the y-axis which happens if and only if $\tan\vartheta = 1/(2k+1)$ for some $k \in \mathbb{N}$. It follows that for any $\tan\vartheta \in \mathbb{Q}$ with $\tan\vartheta \notin \{1/(2k+1)\,;\, k \in \mathbb{N}\}$ there is some $r_0 > 0$ such that *no* component of $M_\vartheta \Omega_r$ meets the y-axis, for $0 < r < r_0$; in other words, in this case all components of $\Omega_{r,\vartheta}$ are discs.

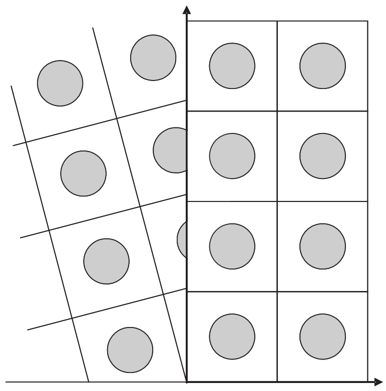

Figure 2.2: The domain $\Omega_{1/4,\pi/8}$ (shaded).

One can prove the following theorem; for more details, see [Hempel, R., Kohlmann, M.: Spectral properties of grain boundaries at small angles of rotation. J. Spectr. Th. 1 (2011) 1–23].

Proposition 2.10. *Let $0 < r < 1/2$ be fixed.*

(1) Each $\mu_k(r)$, $k = 1, 2, \ldots$, is an eigenvalue of infinite multiplicity of $H_{r,\vartheta}$, for all $0 \leq \vartheta \leq \pi/4$. The spectrum of $H_{r,\vartheta}$ is pure point, for all $0 \leq \vartheta \leq \pi/4$.

(2) *For any $\varepsilon > 0$ there is a $\vartheta_\varepsilon = \vartheta_\varepsilon(r) > 0$ such that any interval $(\alpha, \beta) \subset (a, b)$ with $\beta - \alpha \geq \varepsilon$ contains an eigenvalue of $H_{r,\vartheta}$ for any $0 < \vartheta < \vartheta_\varepsilon$.*

(3) *There exists a set $\Theta \subset (0, \pi/2)$ of full measure such that $\sigma(H_{r,\vartheta}) = [\mu_1(r), \infty)$. The eigenvalues different from the $\mu_k(r)$ are of finite multiplicity.*

Remark 2.11. Let $\Lambda := \{\vartheta \in (0, \pi/2)\,;\, \tan\vartheta \in \mathbb{Q}\}$ denote the set of angles where $\tan\vartheta$ is rational; clearly, $\Theta \cap \Lambda = \emptyset$. It is easy to see that $H_{r,\vartheta}$, for $\vartheta \in \Lambda$, has at most a finite number of eigenvalues in (a, b), each of them of infinite multiplicity. Hence we see a drastic change in the spectrum for $\vartheta \in \Lambda$ as compared with $\vartheta \in \Theta$. Furthermore, if $\vartheta \in \Lambda$ with $\tan\vartheta \notin \{1/(2k+1)\,;\, k \in \mathbb{N}\}$, then there is some $r_\vartheta > 0$ such that $\sigma(H_{r,\vartheta}) = \sigma(H_r)$ for all $0 < r < r_\vartheta$.

2.6 Some extensions and remarks

(1) A simple variant of the rotation problem consists in rotations in the left and the right half planes through angles $\vartheta/2$ and $-\vartheta/2$, respectively, i.e., we study

$$\tilde{V}_\vartheta(x, y) = \begin{cases} (V \circ M_{-\vartheta/2})(x, y), & x \geq 0, \\ (V \circ M_{\vartheta/2})(x, y), & x < 0; \end{cases} \tag{2.46}$$

this potential might be rather close to the physical situation shown in Figure 2.1. Here we consider the accompanying translational dislocation potentials

$$\tilde{W}_t(x, y) = \begin{cases} V(x - t/2, y), & x \geq 0, \\ V(x + t/2, y), & x < 0. \end{cases} \tag{5.2}$$

We may then obtain results as in Theorem 2.1 without the use of Birkhoff's theorem: here we only need to take care of the second condition in (2.17) since the horizontal alignment between the left- and right-hand part of V_ϑ on the y-axis is guaranteed by the definition of $\tilde{V}_\vartheta$.

(2) We have shown that the spectral gaps of H fill with spectrum of R_ϑ as $\vartheta \to 0$ in the sense that any interval of length $\varepsilon > 0$ inside a gap of H will contain spectrum of R_ϑ for sufficiently small angles. In general, we do not know whether the spectrum of R_ϑ in the gaps of H_0 is pure point, absolutely continuous or singular continuous. However, there are some special angles where we can exclude singular continuous spectrum: if we assume that $\cos\vartheta$ is a rational number, $\cos\vartheta = q/p$ with $p, q \in \mathbb{N}$, and p and q belong to a Pythagorean triple ($p^2 - q^2 = r^2$ for some $r \in \mathbb{N}$), then V_ϑ has period p in y-direction. In this case, a result in [DS] implies that $\sigma(H_\vartheta)$ has no singular continuous part.

(3) It is natural to ask about higher dimensions. Suppose we are given a potential $V\colon \mathbb{R}^3 \to \mathbb{R}$, periodic with respect to the lattice $\mathbb{Z}^3$. We may then simply consider

rotations of the (x, y)-plane by an angle ϑ, i.e., we let $V_\vartheta(x, y, z) = V(x, y, z)$ in $\{(x, y, z)\,;\, x \geq 0\}$ and $V_\vartheta(x, y, z) = V(M_{-\vartheta}(x, y), z)$ in $\{(x, y, z)\,;\, x < 0\}$, in which case our methods should apply. However, in $\mathbb{R}^3$ there are many other rotations for which our methods may or may not work.

(4) Of course, taking the limit $\vartheta \to 0$ is a mathematical idealization. In real crystals or alloys the lattice and its rotated version have to match up according to certain rules. This is usually only possible for a small number of angles. Related questions in higher dimensions are studied under the name of *coincidence site lattices*.

Chapter 3

The general dislocation problem

In this chapter, we will study dislocation problems on an infinite cylinder $S := \mathbb{R} \times (\mathbb{R}/\mathbb{Z})$ without a periodicity assumption. Given two (bounded and measurable) potentials $V^{(k)} \colon S \to \mathbb{R}$, $k = 1, 2$, the family of *dislocation potentials* is defined by

$$V_t(x,y) = \begin{cases} V^{(1)}(x,y), & x \geq 0, \\ V^{(2)}(x+t,y), & x < 0, \end{cases} \tag{3.1}$$

for $(x,y) \in S$ and $t \in \mathbb{R}$. In the Hilbert space $\mathcal{H} := \mathsf{L}_2(S)$, we let L denote the (unique) self-adjoint extension of $-\Delta$ defined on $\mathsf{C}_\mathrm{c}^\infty(S)$. For each $t \in \mathbb{R}$ the Schrödinger operator $H_t = L + V_t$ describes the energy of an electron on a tube made of the same or two different materials to the left and to the right of the interface $\{0\} \times \mathbb{R}/\mathbb{Z}$. We are interested in the bound states produced by and at this junction where we focus on energies in a spectral gap of H_0. In our main theorem, given below, we will also need the Dirichlet Laplacian $L_{(0,\infty)}$ of $S^+ := (0,\infty) \times \mathbb{R}/\mathbb{Z}$, defined as the Friedrichs extension of $-\Delta$ on $\mathsf{C}_\mathrm{c}^\infty(S^+)$.

Theorem 3.1. *Let $V^{(1)}, V^{(2)} \colon S \to \mathbb{R}$ be bounded and measurable, and let V_t be as in* (3.1)*. Suppose $E \in \mathbb{R}$ is such that*

$$E \notin \sigma(L + V^{(k)}), \qquad k = 1, 2, \tag{3.2}$$

and

$$\inf \sigma_{\mathrm{ess}}(L_{(0,\infty)} + V^{(2)} \restriction S^+) < E. \tag{3.3}$$

Then there exists a sequence $(\tau_j)_{j \in \mathbb{N}} \subset [0,\infty)$ of dislocation parameters such that $E \in \sigma(L + V_{\tau_j})$, and $\tau_j \to \infty$ as $j \to \infty$.

Remark 3.2.

(1) For the case of periodic potentials $V^{(k)}$ on the real line or on $\mathbb{R}^2$ corresponding results had been obtained in the previous chapters. The assumptions in Theorem 3.1 are purely spectral and do not involve any further features of the potentials. In this sense, the occurrence of eigenvalues in gaps for dislocation

problems is not an exception, but it is the rule; to convey this message is the main objective of the present investigations.

(2) In many applications of Theorem 3.1 both $L + V^{(1)}$ and $L + V^{(2)}$ have some essential spectrum below the common gap (a_0, b_0). In the case of half-space problems, however, only one of the operators has essential spectrum below the gap.

(3) We expect the statement of Theorem 3.1 to be true for all $E \in \mathbb{R}$ that satisfy condition (3.3) and $E \notin \sigma_{\mathrm{ess}}(L + V^{(k)})$ for $k = 1, 2$.

(4) Our proof of Theorem 3.1 is based on an approximation on large sections $(-n-t, n) \times \mathbb{R}/\mathbb{Z}$ of the tube, much as in where periodic boundary conditions at the ends $-n-t$ and n have been used. Since the potentials $V^{(k)}$ need not be periodic in x, there is no natural boundary condition at the ends, and we simply take Dirichlet boundary conditions. Of course, this may introduce spurious eigenvalues into the gap that have to be removed by a suitable technique.

The Laplacian L of Thm. 3.1 is unitarily equivalent to the operator L_{per}, defined as the self-adjoint realization of $-\Delta$ on the strip $\mathbb{R} \times (0, 1)$ with periodic boundary conditions in y. We may extend the potentials $V^{(k)}$, $k = 1, 2$, and V_t periodically with respect to the y-variable to all of $\mathbb{R}^2$, and consider the dislocation problem in $\mathbb{R}^2$ with the operators $H_t = -\Delta + V_t$. Then Thm. 3.1 can be used to obtain lower bounds for the integrated density of states inside a gap (a_0, b_0) for certain values of the parameter t.

We finally address the question of continuity of the (discrete) eigenvalues of the family of operators H_t as functions of t. For periodic potentials in one dimension continuity is easy as $V_0 - V_t$ tends to zero in $L_{1,\mathrm{loc,unif}}(S)$, as $t \to 0$. Without periodicity, we now have to face the problem that, no matter how small $t > 0$ might be, $V_0 - V_t$ need not be small on the global scale. Here we use a change of variables to the effect that, in the new coordinates, the potential is altered only in a compact set. This leads to the following basic result.

Theorem 3.3. *Let $V^{(1)}, V^{(2)} \in \mathsf{L}_\infty(S)$ be real-valued, and let $H_t \coloneqq L + V_t$ with V_t as in* (3.1)*. Then the discrete eigenvalues of H_t depend continuously on $t \in \mathbb{R}$. If, in addition, the distributional derivative $\partial_1 V^{(2)}$ is a (signed) Borel measure, the discrete eigenvalues of H_t are (locally) Lipschitz continuous functions of $t \in \mathbb{R}$.*

The second part of the theorem applies in particular if $V^{(2)}$ is of locally bounded variation. Note that Thm. 3.3 also applies to discrete eigenvalues below the essential spectrum of H_t.

3.1 Preliminaries

In this section we introduce notation and collect some basic results related to the dislocation problem.

3.1.1 Notation and Basic Assumptions

The spectral projection associated with a self-adjoint operator T and an interval $I \subset \mathbb{R}$ is denoted as $\mathbb{E}_I(T)$. If T has purely discrete spectrum in I, the number of eigenvalues (counting multiplicities) in I is given by the trace of $\mathbb{E}_I(T)$, denoted as $\operatorname{tr} \mathbb{E}_I(T)$. The Schatten-von Neumann classes will be denoted by $\mathcal{B}_p$, for $1 \le p < \infty$.

Our basic coordinate space is the tube $S = \mathbb{R} \times (\mathbb{R}/\mathbb{Z})$ with the usual (flat) product metric, where $\mathbb{R}/\mathbb{Z} = \frac{1}{2\pi}\mathbb{S}^1$. Let us write $\mathbb{S}' := \mathbb{R}/\mathbb{Z}$ for simplicity of notation. We consider the Sobolev space $\mathsf{H}^1(S)$ with its canonical norm; note that $\mathsf{C}_c^\infty(S)$ is dense in $\mathsf{H}^1(S)$. Equivalently, we could work with the Sobolev space $\mathsf{H}^1_{\mathrm{per}}(\mathbb{R} \times (0,1))$ consisting of functions in $\mathsf{H}^1(\mathbb{R} \times (0,1))$ that are periodic in the y-variable.

In the Hilbert space $\mathsf{L}_2(S)$ we define our basic Laplacian, L, to be the unique (self-adjoint and non-negative) operator associated with the (closed and non-negative) quadratic form

$$\mathsf{H}^1(S) \ni u \mapsto \int_S |\nabla u|^2 \,\mathrm{d}x\,\mathrm{d}y,$$

by the first representation theorem. As on the real line, the Laplacian L is essentially self-adjoint on $\mathsf{C}_c^\infty(S)$. L is unitarily equivalent to the Laplacian $-\Delta$ acting in $\mathsf{L}_2(\mathbb{R} \times (0,1))$ with periodic boundary conditions in the y-variable.

For $M \subset \mathbb{R}$ open we denote by L_M the Friedrichs extension of $-\Delta$, defined on $\mathsf{C}_c^\infty(M \times \mathbb{S}')$, in $\mathsf{L}_2(M \times \mathbb{S}')$; in other words, the form domain of L_M is given as the closure of $\mathsf{C}_c^\infty(M \times \mathbb{S}')$ in $\mathsf{H}^1(S)$. Frequently, M will be an open interval on the real line, or a finite union of such intervals, as in $L_{(\alpha,\beta)}$ for $-\infty \le \alpha < \beta \le \infty$, or in $L_{\mathbb{R}\setminus\{\gamma\}} = L_{(-\infty,\gamma)} \oplus L_{(\gamma,\infty)}$ for $\gamma \in \mathbb{R}$. If $M = (\alpha, \beta)$ for some $-\infty < \alpha < \beta < \infty$, we say that $L_{(\alpha,\beta)}$ satisfies Dirichlet boundary conditions on the lines $\{\alpha\} \times \mathbb{S}'$ and $\{\beta\} \times \mathbb{S}'$.

Given two bounded, measurable functions $V^{(1)}$, $V^{(2)} \colon S \to \mathbb{R}$ we define the Schrödinger operators $H^{(k)} = L + V^{(k)}$, for $k = 1, 2$. Throughout Sections 3.1 and 3.2, we assume $V^{(k)} \ge 0$ for simplicity (and without loss of generality). For $t \in \mathbb{R}$ the dislocation potentials V_t are defined as in (3.1), and we let $H_t = L + V_t$, $t \in \mathbb{R}$, denote the family of dislocation operators.

From a technical point of view, the following three tools are fundamental for our approach:

- decoupling by Dirichlet boundary conditions on circles $\{c\} \times \mathbb{S}'$,
- exponential decay of eigenfunctions,

- a coordinate transformation with respect to the x-variable.

We provide some preliminary facts concerning these tools here. We begin with Dirichlet decoupling.

3.1.2 Dirichlet Decoupling

In this subsection we show how to control the effect of an additional Dirichlet boundary condition on the line $\{0\} \times \mathbb{S}' \subset S$; topologically, $\{0\} \times \mathbb{S}' \subset S$ is a circle. On the strip $\mathbb{R} \times (0,1)$ with periodic boundary conditions the additional Dirichlet boundary condition would be placed on the straight line segment $\{0\} \times (0,1)$. Note that it is essential for our applications later on to have estimates with constants that are uniform for certain classes of potentials.

Lemma 3.4. *Let $0 \leq W \in \mathsf{L}_\infty(S)$, let $H = L + W$ in the Hilbert space $\mathcal{H} = \mathsf{L}_2(S)$, and let $H_D := L_{\mathbb{R}\setminus\{0\}} + W$.*

Then $(H+r)^{-1} - (H_D + r)^{-1}$ is Hilbert-Schmidt for all $r \geq 1$ and there is a constant $C \geq 0$, which is independent of W and r, such that

$$\left\|(H+r)^{-1} - (H_D+r)^{-1}\right\|_{\mathcal{B}_2(\mathcal{H})} \leq C, \qquad r \geq 1. \tag{3.4}$$

Estimates of type (3.4) are well-known and have been of great use in spectral and in scattering theory. Similar estimates hold for finite tubes $(-n,n) \times \mathbb{S}'$ where we compare $L_{(-n,n)}$ and $L_{(-n,n)\setminus\{0\}} = L_{(-n,0)} \oplus L_{(0,n)}$.

Lemma 3.5. *Let $0 \leq W \in \mathsf{L}_\infty(S)$ and let $L_{(-n,n)}$ and $L_{(-n,n)\setminus\{0\}}$ be as above. Then $(L_{(-n,n)} + W + r)^{-1} - (L_{(-n,n)\setminus\{0\}} + W + r)^{-1}$ is Hilbert-Schmidt for $r \geq 1$ and we have an estimate*

$$\left\|(L_{(-n,n)} + W + r)^{-1} - (L_{(-n,n)\setminus\{0\}} + W + r)^{-1}\right\|_{\mathcal{B}_2(\mathcal{H})} \leq C,$$

with a constant C independent of r and W.

Proof. Exercise 11. □

It is easy to generalize the above results to situations where we add in Dirichlet boundary conditions on several lines of the type $\{x_0\} \times \mathbb{S}'$. This immediately gives a simple proof for the invariance of the essential spectrum.

Proposition 3.6. *For $k = 1,2$, let $V^{(k)} \in \mathsf{L}_\infty(S)$ and define $H^{(k)}$ and H_t as above. In addition, let $H_+^{(1)} := L_{(0,\infty)} + V^{(1)}$ and $H_-^{(2)} := L_{(-\infty,0)} + V^{(2)}$. We then have*

$$\sigma_{\text{ess}}(H_t) = \sigma_{\text{ess}}(H_+^{(1)}) \cup \sigma_{\text{ess}}(H_-^{(2)}) \subset \sigma_{\text{ess}}(H^{(1)}) \cup \sigma_{\text{ess}}(H^{(2)}), \qquad t \in \mathbb{R}. \tag{3.5}$$

Proof. For $t \geq 0$, let $H_{t,\mathrm{dec}}$ denote the operator obtained from H_t by the insertion of Dirichlet boundary conditions on the lines $\{0\} \times \mathbb{S}'$ and $\{-t\} \times \mathbb{S}'$. By Lemma 3.4, $(H_t + 1)^{-1} - (H_{t,\mathrm{dec}} + 1)^{-1}$ is compact and so H_t and $H_{t,\mathrm{dec}}$ have the same essential spectrum. The part of $H_{t,\mathrm{dec}}$ to the left of $-t$ is unitarily equivalent to $H_-^{(2)}$, and the part of $H_{t,\mathrm{dec}}$ associated with the interval $(-t, 0)$ has compact resolvent. Thus $\sigma_{\mathrm{ess}}(H_{t,\mathrm{dec}}) = \sigma_{\mathrm{ess}}(H_{0,\mathrm{dec}}) = \sigma_{\mathrm{ess}}(H_+^{(1)}) \cup \sigma_{\mathrm{ess}}(H_-^{(2)})$. This proves the equality in (3.5). The inclusion stated in (3.5) is immediate from Lemma 3.4. □

3.1.3 Exponential Decay of Eigenfunctions

The following contains our basic exponential decay estimate. It is of importance for the applications we are having in mind that the bound of Lemma 3.7 below is independent of W within the class of bounded, non-negative potentials with a given spectral gap (a_0, b_0). We let χ_k denote the characteristic function of the set $[-k, k] \times \mathbb{S}' \subset S$, for brevity. We also omit a proof for the convenience of the reader.

Lemma 3.7. *For $0 \leq a_0 < a < b < b_0$ given there exist constants $C \geq 0$ and $\gamma > 0$ such that for all $0 \leq W \in \mathsf{L}_\infty(S)$ with $\sigma(L + W) \cap (a_0, b_0) = \emptyset$ we have*

$$\|(1 - \chi_k)u\| \leq C e^{-\gamma k} \|u\|, \qquad k \in \mathbb{N},$$

for all eigenfunctions u of $L_{\mathbb{R}\setminus\{0\}} + W$ that are associated with an eigenvalue $\lambda \in [a, b]$.

The following lemma gives an upper bound for the number of eigenvalues that are moved into a compact subset $[a, b]$ of a spectral gap (a_0, b_0) upon enforcing a Dirichlet boundary condition on the line $\{0\} \times \mathbb{S}'$. Again, it is important that the bound is *independent* of the potential W, provided $W \geq 0$.

Lemma 3.8. *For numbers $a_0 < a < b < b_0 \in \mathbb{R}$ given there exists a constant $c \geq 0$ with the following property: If $0 \leq W \in \mathsf{L}_\infty(S)$ satisfies $\sigma(L + W) \cap (a_0, b_0) = \emptyset$, then*

$$\operatorname{tr} \mathbb{E}_{[a,b]}(L_{\mathbb{R}\setminus\{0\}} + W) \leq c.$$

3.1.4 Transformation of Coordinates

Some additional insight can be gained by using a transformation of coordinates which, in a sense, "undoes" the effect of the dislocation outside a finite section of the tube S. In this way, the dislocation problem can be viewed as a perturbation which acts in a compact subset of S only. To this end, we provide (smooth) diffeomorphisms $\varphi_t \colon \mathbb{R} \to \mathbb{R}$ of class C^∞ with the additional properties that

$$\varphi_t(x) = x, \quad x \geq 0, \qquad \varphi_t(x) = x - t, \quad x \leq -2;$$

we also require that there is a constant $C \geq 0$ s.th.

$$\max_{x\in\mathbb{R}} |\varphi_t(x) - x|, \quad \max_{x\in\mathbb{R}} |\varphi_t'(x) - 1|, \quad \max_{x\in\mathbb{R}} |\varphi_t''(x)| \leq Ct, \qquad t \in [0, 2].$$

In Exercise 14, it will be shown that, for $0 \le t \le 1$, the dislocation operators H_t are unitarily equivalent to (s.a.) operators $\hat{H}_t$ acting in $\mathsf{L}_2(S)$ with domain $D(\hat{H}_t) = D(L)$ where the quadratic form of $\hat{H}_t$ is given by

$$\hat{H}_t[u,u] := \int_S \left(\frac{1}{(\varphi_t')^2} |\partial_1 u|^2 + |\partial_2 u|^2 - \frac{\varphi_t''}{(\varphi_t')^3} \operatorname{Re}(\bar{u}\partial_1 u) + \frac{(\varphi_t'')^2}{4(\varphi_t')^4} |u|^2 \right) \mathrm{d}x\,\mathrm{d}y \\ + \int_S V_t(\varphi_t(x), y)|u|^2 \,\mathrm{d}x\,\mathrm{d}y;$$

here $\hat{H}_0 = H_0 = H$. Note that $\hat{H}_t - H_0$ has support in the compact set $\{-2 \le x \le 0\}$. In other words, the family $(\hat{H}_t)_{0\le t\le 1}$ gives an equivalent description of the dislocation problem where the perturbation is now restricted to the bounded set $\{(x,y) \in S;\ -2 \le x \le 0\}$.

One can show the family $(\hat{H}_t)_{0\le t\le 1}$ enjoys the following properties:
(1) The mapping $[0,1] \ni t \mapsto (\hat{H}_t + 1)^{-1}$ is norm-continuous.
(2) For $t, t' \in [0,1]$, the resolvent difference $(\hat{H}_t + 1)^{-1} - (\hat{H}_{t'} + 1)^{-1}$ is compact. Here, the result of Exercise 12 is involved crucially.

It follows from (2) that the essential spectrum of $\hat{H}_t$ is stable, and then the same property holds for the family $(H_t)_{0\le t\le 1}$. Property (1) implies that the spectrum of $\hat{H}_t$ depends continuously on t in the usual Hausdorff-metric on the real line, and then the same holds for the family $(H_t)_{0\le t\le 1}$. This provides a proof of the first part of Theorem 3.3.

3.2 The main result

In this section we give a proof of Theorem 3.1. We consider some $E \in \mathbb{R}$ satisfying the assumptions (3.2) and (3.3) of Thm. 3.1. It follows from condition (3.2) that there is an $\alpha > 0$ such that

$$\operatorname{dist}(E, \sigma(L + V^{(k)})) \ge 2\alpha, \qquad k = 1, 2;$$

E and α will be kept fixed throughout this section. If it happens that E is an eigenvalue of $H_0 = L + V_0$ we set $\tau_1 := 0$ and consider H_1 instead of H_0. We may therefore assume in the sequel that $E \notin \sigma(H_0)$. We now fix some $0 < \beta \le 2\alpha/3$ such that

$$\operatorname{dist}(E, \sigma(H_0)) \ge 3\beta. \tag{3.6}$$

We find solutions of suitable approximating problems, and then pass to the limit. The basic idea is to restrict the problem to finite sections of the tube S of the form $(-n-t, n) \times \mathbb{S}'$, as in the chapters before where S is a strip and the potential V is periodic. In the previous considerations, periodic boundary conditions at the ends of the finite strip worked nicely, but for non-periodic potentials there is no natural choice of boundary conditions on the lines $\{\pm n\} \times \mathbb{S}'$ that would keep the interval

$(E-\beta, E+\beta)$ free of spectrum of the operators $H_{n,0} = L_{(-n,n)} + V_0$ and we have to resort to a more complicated construction.

3.2.1 The Approximating Problems

We first introduce "correction terms" in the form of projections, sandwiched between suitable cut-offs. While we have two interacting Dirichlet boundaries, we prefer a construction where the correction term at the left end does not depend on the correction term at the right end. Let

$$\begin{aligned} H_n^+ &= L_{(-\infty,n)} + V^{(1)} \text{ in } \mathsf{L}_2((-\infty,n)\times\mathbb{S}'),\\ H_n^- &= L_{(-n,\infty)} + V^{(2)} \text{ in } \mathsf{L}_2((-n,\infty)\times\mathbb{S}'), \end{aligned}$$

for $n \in \mathbb{N}$, where we have chosen the upper indices $\pm$ of $H_n^\pm$ in reference to the Dirichlet boundary condition on the lines $\{\pm n\}\times\mathbb{S}'$. As in Prop. 3.6, we have $\sigma_{\mathrm{ess}}(H_n^+) \subset \sigma_{\mathrm{ess}}(H^{(1)})$ and $\sigma_{\mathrm{ess}}(H_n^-) \subset \sigma_{\mathrm{ess}}(H^{(2)})$ so that $(E-3\beta, E+3\beta)$ is a gap in the essential spectrum of $H_n^\pm$. We are now going to construct a family of operators $\tilde{H}_{n,t}$ on $(-n-t,n)\times\mathbb{S}'$ that will serve as approximations to H_t and which enjoy the property that the interval $(E-\beta,E+\beta)$ is free of spectrum of $\tilde{H}_{n,0}$.

Let $\Phi^\pm_{n,k}$, $k=1,\ldots,J_n^\pm$, denote a (maximal) orthonormal set of eigenfunctions of $H_n^\pm$ corresponding to its eigenvalues in $[E-2\beta,E+2\beta]$. By Lemma 3.8, there is a constant c_0 such that $J_n^\pm \le c_0$ for all n; here we apply Lemma 3.8 twice, with the choice $a_0 := E-3\beta$, $a := E-2\beta$, $b := E+2\beta$, $b_0 := E+3\beta$, and $W := V^{(1)}(.+n)$ or $W := V^{(2)}(.-n)$, respectively.

Next, we introduce the projections $P_n^\pm$ onto the span of the $\Phi^\pm_{n,k}$, given by

$$P_n^\pm = \mathbb{E}_{[E-2\beta,E+2\beta]}(H_n^\pm).$$

As a consequence,

$$\sigma(H_n^\pm + 4\beta P_n^\pm) \cap [E-2\beta,E+2\beta] = \emptyset. \tag{3.7}$$

Here the eigenfunctions $\Phi^\pm_{n,k}$ are localized near $\{\pm n\}\times\mathbb{S}'$ and decay (exponentially) as x increases or decreases from $\pm n$, cf. Lemma 3.7. We are now going to make this more precise.

Let us first introduce some cut-off functions. Let $\chi_1^+ \in \mathsf{C}^\infty(-\infty,1)$ with $0 \le \chi_1^+ \le 1$, $\chi_1^+(x) = 1$ for $x > 3/4$, and $\chi_1^+(x) = 0$ for $x < 1/2$, be given. Now set $\chi_n^+(x) = \chi_1(x/n)$, so that $\chi_n^+ \in \mathsf{C}^\infty(-\infty,n)$, $\chi_n^+(x) = 1$ for $x > 3n/4$, and $\chi_n^+(x) = 0$ for $x < n/2$. We define $\chi_n^- \in \mathsf{C}^\infty(-n,\infty)$ analogously by setting $\chi_n^-(x) = \chi_n^+(-x)$. Furthermore, choose $\varphi_1 \in \mathsf{C}_c^\infty(-1/2,1/2)$ with $0 \le \varphi_1 \le 1$ and $\varphi_1(x) = 1$ for $|x| < 1/4$, and set $\varphi_n(x) = \varphi_1(x/n)$ and $\psi_n = 1-\varphi_n$. Finally, we decompose $\psi_n = \psi_n^- + \psi_n^+$ and note that $\psi_n^\pm\chi_n^\pm = \chi_n^\pm$. By Lemma 3.7 there are constants $c \ge 0$ and $n_0 \in \mathbb{N}$ such that

$$\left\|(1-\chi_n^\pm)\Phi^\pm_{n,k}\right\| \le c/n, \qquad n \ge n_0,$$

and we infer that there is a constant $C \geq 0$ such that

$$\left\|\chi_n^\pm P_n^\pm \chi_n^\pm - P_n^\pm\right\| \leq \frac{C}{n}; \tag{3.8}$$

in fact, a stronger estimate of the form $\|\chi_n^\pm P_n^\pm \chi_n^\pm - P_n^\pm\| \leq C' e^{-\gamma n}$, for some $\gamma > 0$, holds true. We now define

$$\tilde{H}_n^\pm = H_n^\pm + 4\beta \chi_n^\pm P_n^\pm \chi_n^\pm$$

and observe that, by (3.7) and (3.8),

$$\sigma(\tilde{H}_n^\pm) \cap [E-\beta, E+\beta] = \emptyset,$$

for n large. In particular, for any $u \in D(\tilde{H}_n^\pm) = D(H_n^\pm)$ we have

$$\|u\| \leq \frac{1}{\beta}\left\|(\tilde{H}_n^\pm - E)u\right\|. \tag{3.9}$$

Now the dislocation enters the game: let $T_t(x,y) = (x+t, y)$, for $(x,y) \in S$, and define

$$P_{n,t}^- = \sum_{k \in J_n^-} \left\langle\,.\,, \Phi_{n,k}^- \circ T_t\right\rangle \Phi_{n,k}^- \circ T_t,$$

as well as $\chi_{n,t}^- := \chi_n^- \circ T_t$. Finally, let

$$\mathcal{P}_{n,t} = 4\beta\left(\chi_n^+ P_n^+ \chi_n^+ + \chi_{n,t}^- P_{n,t}^- \chi_{n,t}^-\right)$$

and

$$\tilde{H}_{n,t} = L_{(-n-t,n)} + V_t + \mathcal{P}_{n,t}$$

in $\mathsf{L}_2((-n-t,n) \times \mathbb{S}')$. The operators $\tilde{H}_{n,t}$ are the principal players in our approximating problems. We first establish that the operators $\tilde{H}_{n,0}$ have no spectrum in the interval $[E-\beta, E+\beta]$, for n large.

Lemma 3.9. *Let $E \in \mathbb{R} \setminus \sigma(H_0)$ satisfy condition* (3.2) *of Thm. 3.1 and let β be as in* (3.6). *Then there is an $n_0 \in \mathbb{N}$ such that*

$$\sigma(\tilde{H}_{n,0}) \cap (E-\beta, E+\beta) = \emptyset, \qquad n \geq n_0.$$

Proof. Else there exists a sequence $n_j \to \infty$ and there exist $E_j \in [E-\beta, E+\beta]$ such that E_j is an eigenvalue of $\tilde{H}_{n_j,0}$, for $j \in \mathbb{N}$. Let u_{n_j} denote an associated normalized eigenfunction. With the cut-off functions φ_k and $\psi_k^\pm$ defined above, we see that $\varphi_{n_j/4} u_{n_j} \in D(H_0)$ and $\psi_{n_j/4}^\pm u_{n_j} \in D(\tilde{H}_{n_j}^\pm)$ with estimates

$$\left\|(H_0 - E_j)(\varphi_{n_j/4} u_{n_j})\right\| \leq c/n_j, \qquad \left\|(\tilde{H}_{n_j}^\pm - E_j)(\psi_{n_j/4}^\pm u_{n_j})\right\| \leq c/n_j, \tag{3.10}$$

for j large; here $c \geq 0$ is a suitable constant. Since $\sigma(H_0) \cap (E-2\beta, E+2\beta) = \emptyset$ and $E_j \in [E-\beta, E+\beta]$, we have $\|(H_0 - E_j)u\| \geq \beta\|u\|$ for all $u \in D(H_0)$, so that $\varphi_{n_j/4} u_{n_j} \to 0$ as $j \to \infty$. Similarly, the second estimate in (3.10) and (3.9) imply that $\psi_{n_j/4}^\pm u_{n_j} \to 0$, as $j \to \infty$. Therefore $u_{n_j} \to 0$ as $j \to \infty$, in contradiction to $\left\|u_{n_j}\right\| = 1$. $\square$

3.2.2 Solution of the Approximating Problems.

We are now going to show that, for large $n \in \mathbb{N}$, there exist parameters $t_n \geq 0$ such that E is an eigenvalue of $\tilde{H}_{n,t_n}$. Since all the operators involved have purely discrete spectrum we can use a simple eigenvalue counting argument.

Proposition 3.10. *Let $E \in \mathbb{R}\setminus\sigma(H_0)$ satisfy conditions* (3.2) *and* (3.3) *of Theorem 3.1. Then there are $n_0 \in \mathbb{N}$ and $\gamma_0 > 0$ such that for any $n \in \mathbb{N}$ with $n \geq n_0$ there exists $0 < t_n \leq \gamma_0$ such that E is an eigenvalue of $\tilde{H}_{n,t_n}$.*

In preparation for the proof, we introduce variants of our operators with Dirichlet boundary conditions on suitable lines. Let $\tilde{H}_{n,t;\mathrm{dec}}$ denote the operator $\tilde{H}_{n,t}$ with additional DBCs on the lines $\{0\} \times \mathbb{S}'$ and $\{-t\} \times \mathbb{S}'$; note that—by virtue of the cut-offs χ_n^+ and $\chi_{n,t}^-$—the non-local operators $\mathcal{P}_{n,t}$ are not affected by these boundary conditions. For $n \geq n_0(t)$ the operators $\tilde{H}_{n,t;\mathrm{dec}}$ can be written as direct sums

$$\tilde{H}_{n,t;\mathrm{dec}} = \tilde{h}_{n,t;1} \oplus h_{t;2} \oplus \tilde{h}_{n;3},$$

with

$$\tilde{h}_{n,t;1} := L_{(-n-t,-t)} + V_t + 4\beta\chi_{n,t}^- P_{n,t}^- \chi_{n,t}^-,$$

acting in $\mathsf{L}_2((-n-t,-t) \times \mathbb{S}')$ with DBCs on $\{-n-t\} \times \mathbb{S}'$ and on $\{-t\} \times \mathbb{S}'$,

$$h_{t;2} := L_{(-t,0)} + V_t$$

acting in $\mathsf{L}_2((-t,0) \times \mathbb{S}')$ with DBCs on $\{-t\} \times \mathbb{S}'$ and on $\{0\} \times \mathbb{S}'$, and, finally,

$$\tilde{h}_{n;3} := L_{(0,n)} + V^{(1)} + 4\beta\chi_n^+ P_n^+ \chi_n^+,$$

acting in $\mathsf{L}_2((0,n) \times \mathbb{S}')$ with DBCs on $\{0\} \times \mathbb{S}'$ and on $\{n\} \times \mathbb{S}'$.

We now collect some properties of the operators $\tilde{H}_{n,t;\mathrm{dec}}$ that we need in the proof of Proposition 3.10.

(1) For $t = 0$ we have

$$\begin{aligned}\tilde{H}_{n,0;\mathrm{dec}} &= \tilde{h}_{n,0;1} \oplus \tilde{h}_{n;3} \\ &= (L_{(-n,0)} + V^{(2)} + 4\beta\chi_n^- P_n^- \chi_n^-) \oplus (L_{(0,n)} + V^{(1)} + 4\beta\chi_n^+ P_n^+ \chi_n^+).\end{aligned}$$

The following lemma compares the number of eigenvalues below E for the operators $\tilde{H}_{n,0}$ and $\tilde{H}_{n,0;\mathrm{dec}}$.

Lemma 3.11. *Let E and β satisfy* (3.6)*, let $\tilde{H}_{n,0}$ and $\tilde{H}_{n,t;\mathrm{dec}}$ be as above, and let n_0 as in Lemma 3.9. Then there is a constant $c_0 \geq 0$ such that*

$$\operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,0}) \geq \operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,0;\mathrm{dec}}) \geq \operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,0}) - c_0, \qquad n \geq n_0.$$

In the proof of Lemma 3.11 we use a proposition, based on the Birman-Schwinger principle to control the spectral shift across E, produced by the Dirichlet boundary condition on $\{0\} \times \mathbb{S}'$. Recall that $\mathcal{B}_p$ denotes the p-th Schatten-von Neumann class, for $1 \leq p < \infty$.

Proposition 3.12. *Let $1 \leq T \leq S$ be self-adjoint operators with compact resolvent in the Hilbert-space $\mathcal{H}$, and suppose that $T^{-1} - S^{-1} \in \mathcal{B}_p(\mathcal{H})$ for some $p \in [1, \infty)$. Then for any $E \in \mathbb{R} \setminus \sigma(T)$ we have*

$$\operatorname{tr} \mathbb{E}_{(-\infty,E)}(S) \geq \operatorname{tr} \mathbb{E}_{(-\infty,E)}(T) - \operatorname{dist}(E, \sigma(T))^{-p} \left\| T^{-1} - S^{-1} \right\|_{\mathcal{B}_p}^p .$$

Proof. The proof is immediate from Proposition 1.1 in [H92] with $A := (T+1)^{-1}$, $B := (S+1)^{-1}$, and $\eta := (E+1)^{-1}$. ☐

Proof (of Lemma 3.11). The first inequality follows immediately from $\tilde{H}_{n,0;\text{dec}} \geq \tilde{H}_{n,0}$. To prove the second inequality, we apply Prop. 3.12 with $T := \tilde{H}_{n,0} + 1$, $S := \tilde{H}_{n,0,\text{dec}} + 1$, and $p = 2$. Here $(H_{n,0} + 1)^{-1} - (H_{n,0,\text{dec}} + 1)^{-1}$ is Hilbert-Schmidt by Lemma 3.5 with a bound c_1 on the HS-norm which is independent of n. Simple perturbational arguments ([H92, Lemma 1.4]) yield that there exists a constant $c_2 \geq 0$ such that

$$\left\| (\tilde{H}_{n,0} + 1)^{-1} - (\tilde{H}_{n,0,\text{dec}} + 1)^{-1} \right\|_{\mathcal{B}_2} \leq c_2, \qquad n \geq n_0.$$

Now Prop. 3.12 implies

$$\operatorname{tr} \mathbb{E}_{(-\infty,E)}(\tilde{H}_{n,0,\text{dec}}) \geq \operatorname{tr} \mathbb{E}_{(-\infty,E)}(\tilde{H}_{n,0}) - \beta^{-2} c_2^2;$$

here the left hand side is enlarged if we replace $\mathbb{E}_{(-\infty,E)}$ with $\mathbb{E}_{(-\infty,E]}$ while the right hand side remains unchanged under this replacement since $E \notin \sigma(\tilde{H}_{n,0})$. ☐

(2) The operator $\tilde{h}_{n,t;1}$ is unitarily equivalent to $\tilde{h}_{n,0;1}$ via a right-translation through t so that

$$\operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{h}_{n,t;1}) + \operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{h}_{n;3}) = \operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,0;\text{dec}}). \tag{3.11}$$

(3) The operators $h_{t;2}$ are unitarily equivalent to $L_{(0,t)} + V^{(2)} \restriction (0,t)$ for all $t > 0$ by a right translation and we have the following lemma.

Lemma 3.13. *Let $h_{t;2}$ as above and let E and $V^{(2)}$ satisfy condition* (3.3)*. Then*

$$\operatorname{tr} \mathbb{E}_{(-\infty,E)}(h_{t;2}) \to \infty, \qquad t \to \infty. \tag{3.12}$$

For the proof we prepare a lemma.

Lemma 3.14. *Let A and A_n, for $n \in \mathbb{N}$, be bounded, symmetric operators in some Hilbert space and suppose that $A_n \to A$ strongly. Then, for any $\lambda_0 \in \sigma_{\text{ess}}(A)$ and any $\varepsilon > 0$ we have* $\operatorname{tr} \mathbb{E}_{(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)}(A_n) \to \infty$ *as $n \to \infty$.*

In Lemma 3.14 we allow for $\operatorname{tr} \mathbb{E}_{(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)}(A_n) = \infty$; a precise statement would read as follows: For any $k \in \mathbb{N}$ there exists $n_0 \in \mathbb{N}$ such that $\operatorname{tr} \mathbb{E}_{(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)}(A_n) \in [k, \infty]$ for all $n \geq n_0$.

Proof. Assume for a contradiction that there exist $\lambda_0 \in \sigma_{\mathrm{ess}}(A)$, $k_0 \in \mathbb{N}$, and a sequence $(n_j) \subset \mathbb{N}$ with $n_j \to \infty$, as $j \to \infty$, such that $\operatorname{tr} \mathbb{E}_{(\lambda_0-\varepsilon,\lambda_0+\varepsilon)}(A_{n_j}) \le k_0$ for all $j \in \mathbb{N}$.

Let $0 < \varepsilon' < \varepsilon$ and choose a continuous function $f\colon \mathbb{R} \to [0,1]$ such that $f(x) = 1$ for $|x - \lambda_0| \le \varepsilon'$ and $f(x) = 0$ for $|x - \lambda_0| \ge \varepsilon$. By routine arguments, it follows from the assumptions that $p(A_n) \to p(A)$ strongly for all real-valued polynomials and then that $f(A_n) \to f(A)$ strongly; here we also use that the norms $\|A_n\|$ form a bounded sequence.

There exists an ONS $\{u_1, \ldots, u_{k_0+1}\} \subset \operatorname{Ran} \mathbb{E}_{(\lambda_0-\varepsilon',\lambda_0+\varepsilon')}(A)$. As $\chi_{(\lambda_0-\varepsilon,\lambda_0+\varepsilon)} \ge f \ge 0$, monotonicity of the trace yields

$$\operatorname{tr} \mathbb{E}_{(\lambda_0-\varepsilon,\lambda_0+\varepsilon)}(A_{n_j}) \ge \operatorname{tr} f(A_{n_j}) \ge \sum_{m=1}^{k_0+1} \langle f(A_{n_j})u_m, u_m \rangle$$

with $\sum_{m=1}^{k_0+1} \langle f(A_{n_j})u_m, u_m \rangle \to \sum_{m=1}^{k_0+1} \langle f(A)u_m, u_m \rangle = k_0 + 1$, as $j \to \infty$. $\square$

Proof (of Lemma 3.13). Since $h_{t;2}$ and $L_{(0,t)} + V^{(2)}$ are unitarily equivalent, we only have to show that $\operatorname{tr} \mathbb{E}_{(-\infty,E)}(L_{(0,t)} + V^{(2)}) \to \infty$ as $t \to \infty$. Here we may use Lemma 3.14, applied to the operators

$$A \coloneqq (L_{(0,\infty)} + V^{(2)} + 1)^{-1}, \qquad A_t \coloneqq (L_{(0,t)} + V^{(2)} + 1)^{-1} \oplus 0,$$

with the operator 0 acting in $\mathsf{L}_2((t,\infty) \times \mathbb{S}')$. Indeed, it follows from a result in [S78] that $A_t \to A$ strongly, as $t \to \infty$. $\square$

Let us note as an aside that there is a kind of converse to the statement of Lemma 3.13: If $\eta < \inf \sigma_{\mathrm{ess}}(L_{(0,\infty)} + V^{(2)})$, then min-max and $L_{(0,t)} + V^{(2)} \ge L_{(0,\infty)} + V^{(2)}$ imply that

$$\operatorname{tr} \mathbb{E}_{(-\infty,\eta]}(L_{(0,t)} + V^{(2)}) \le \operatorname{tr} \mathbb{E}_{(-\infty,\eta]}(L_{(0,\infty)} + V^{(2)}) < \infty, \qquad t > 0,$$

and thus $\operatorname{tr} \mathbb{E}_{(-\infty,\eta]}(L_{(0,t)} + V^{(2)})$ is a bounded function of $t > 0$.

We are now ready for the proof of Proposition 3.10.

Proof of Prop. 3.10. Let $E \in (a,b) \setminus \sigma(H_0)$. By Lemma 3.9 there exist $\beta > 0$ and $n_0 \in \mathbb{N}$ such that

$$(E - \beta, E + \beta) \cap \sigma(\tilde{H}_{n,0}) = \emptyset, \qquad n \ge n_0.$$

Adding in Dirichlet boundary conditions raises eigenvalues and we thus have

$$\begin{aligned}
\operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,t}) &\ge \operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,t;\mathrm{dec}}) \\
&= \operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{h}_{n,t;1}) + \operatorname{tr} \mathbb{E}_{(-\infty,E]}(h_{t;2}) + \operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{h}_{n;3}) \\
&= \operatorname{tr} \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,0;\mathrm{dec}}) + \operatorname{tr} \mathbb{E}_{(-\infty,E]}(h_{t;2}),
\end{aligned}$$

where we have used (3.11) in the last step. It now follows from Lemma 3.11 that

$$\operatorname{tr}\, \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,t}) \geq \operatorname{tr}\, \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,0}) - c_0 + \operatorname{tr}\, \mathbb{E}_{(-\infty,E]}(h_{t;2}),$$

with the constant c_0 from Lemma 3.11. Since $V^{(2)}$ satisfies condition (3.3), Lemma 3.13 implies that there exists $\gamma_0 > 0$ such that $\operatorname{tr}\, \mathbb{E}_{(-\infty,E]}(h_{\gamma_0;2}) > c_0$ and we conclude that

$$\operatorname{tr}\, \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,\gamma_0}) > \operatorname{tr}\, \mathbb{E}_{(-\infty,E]}(\tilde{H}_{n,0}), \qquad n \geq n_0. \tag{3.13}$$

The operators $\tilde{H}_{n,t}$ have purely discrete spectrum and their eigenvalues depend continuously on $t \geq 0$, as can be easily seen by arguments similar to the ones used for the periodic problem. Therefore, (3.13) implies that at least one eigenvalue of $\tilde{H}_{n,t}$ has crossed E at some $0 < t_n \leq \gamma_0$, and we are done. □

The above Prop. 3.10 shows that there exists a bounded sequence of parameters t_n such that E is an eigenvalue of $\tilde{H}_{n,t_n}$. Then there is a convergent subsequence $t_{n_j} \to \bar{t}$, as $j \to \infty$, and we expect that E is an eigenvalue of $H_{\bar{t}}$.

Lemma 3.15. *Suppose we are given sequences $(t_n) \subset [0, \infty)$ and $(E_n) \subset [E-\beta, E+\beta]$ with $t_n \to \bar{t}$ and $E_n \to E$, as $n \to \infty$, with the property that E_n is an eigenvalue of $\tilde{H}_{n,t_n}$ for $n \geq n_0$. Then E is an eigenvalue of $H_{\bar{t}}$.*

Proof. Exercise 16. □

We are now ready for the proof of Thm. 3.1.

Proof of Theorem 3.1. If $E \in \sigma(H_0)$, let $\tau_1 := 0$. Else Prop. 3.10 and Lemma 3.15 directly yield a $\tau_1 \geq 0$ such that $E \in \sigma(H_{\tau_1})$; in this case we would in fact know that $\tau_1 > 0$.

If E happens to be an eigenvalue of H_{τ_1+1}, we let $\tau_2 := \tau_1 + 1$. Else we replace $V^{(2)}$ with $V^{(2)} \circ T_{\tau_1+1}$, to obtain some $\tau_2 \geq \tau_1 + 1$ with $E \in \sigma(H_{\tau_2})$, and so on. □

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