A VARIATIONAL APPROACH TO DISLOCATION PROBLEMS 
FOR PERIODIC SCHRÖDINGER OPERATORS

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Abstract. As a simple model for lattice defects like grain boundaries in solid 
state physics we consider potentials which are obtained from a periodic potential 
\( V = V(x, y) \) on \( \mathbb{R}^2 \) with period lattice \( \mathbb{Z}^2 \) by setting \( W_t(x, y) = V(x + t, y) \) for \( x < 0 \) and \( W_t(x, y) = V(x, y) \) for \( x \geq 0 \), for \( t \in [0, 1] \). For Lipschitz-
continuous \( V \) it is shown that the Schrödinger operators \( H_t = -\Delta + W_t \) have 
spectrum (surface states) in the spectral gaps of \( H_0 \), for suitable \( t \in (0, 1) \). We 
also discuss the density of these surface states as compared to the density of 
the bulk. Our approach is variational and it is first applied to the well-known 
dislocation problem [K1, K2] on the real line. We then proceed to the dis-
location problem for an infinite strip and for the plane. In an appendix, we 
discuss regularity properties of the eigenvalue branches in the one-dimensional 
dislocation problem for suitable classes of potentials.

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: there are defects 
which leave the lattice unchanged (like impurities or vacancies), and there are 
more serious “geometric” defects of the lattice itself, cf. [AM], which may involve 
translations and rotation of portions of the lattice. Such lattice dislocations occur, 
in particular, at grain boundaries in alloys. These models 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, 
 cf. [DS]: there is a periodic potential \( V: \mathbb{R}^d \to \mathbb{R} \) with period lattice \( \mathbb{Z}^d \) and a 
Euclidean transformation \( T: \mathbb{R}^d \to \mathbb{R}^d \) 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. In the present paper, we discuss the case \( d = 2 \) (where 
the coordinates are denoted by \( x \) and \( y \)) and we will mainly focus on translation 
in the \( x \)-direction. In a forthcoming companion paper [HK] we will then study 
some aspects of the rotation problem where we take the given periodic potential 

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V in the right half-plane and a rotated version \( V \circ M_\vartheta \) in the left half-plane with \( M_\vartheta \) denoting rotation by the angle \( \vartheta \); some results from the present paper will be essential for [HK].

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

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

for \( t \in [0, 1] \). The (self-adjoint) operator \( H_t := -\frac{d^2}{dx^2} + W_t \) is called the dislocation operator, \( t \) the dislocation parameter. There is quite a number of results available on this problem: it is well known and easy to see that the essential spectrum of \( H_t \) does not depend on \( t \) for \( 0 \leq t \leq 1 \); also \( H_t \) cannot have any embedded eigenvalues. Furthermore, there is no singular continuous spectrum, cf. [DS]. For \( 0 < t < 1 \), the operators \( H_t \) may have bound states (discrete eigenvalues) located in the gaps of the essential spectrum. These eigenvalues and the corresponding resonances have been studied by Korotyaev [K1, K2] in great detail, using powerful results from analytic function theory which are specific to the one-dimensional, periodic case. While, predictably, our results for the one-dimensional periodic case are weaker than Korotyaev’s, our method of proof is very elementary and can be generalized in several directions; most importantly, we can apply our techniques to dislocation problems in dimensions greater than 1. In one dimension, we also give a more systematic treatment of regularity properties of the eigenvalue “branches”; in particular, it is shown that the eigenvalue branches are Lipschitz-continuous if \( V \) is (locally) of bounded variation.

The one-dimensional dislocation problem is mainly included to introduce and test our variational approach which is inspired by [DH, ADH]: we use approximations by problems on intervals \((-n - t, n)\) with periodic boundary conditions where it is easy to control the spectral flow, and let \( n \) tend to \( \infty \). This idea can be adapted to the study of the translation problem for the strip \( \Sigma := \mathbb{R} \times (0, 1) \) in \( \mathbb{R}^2 \) with periodic boundary conditions in the \( y \)-variable, say. In \( \mathbb{R}^2 \), we consider dislocation potentials \( W_t \) defined by

\[
W_t(x, y) := \begin{cases} 
V(x, y), & x \geq 0, \\
V(x + t, y), & x < 0,
\end{cases}
\]

for \( t \in [0, 1] \). On the strip \( \Sigma \) we obtain existence results for eigenvalues of \( S_t := -\Delta + W_t \) in the spectral gaps of \( S_0 \). From that we easily derive that \( D_t := -\Delta + W_t \), acting in \( L^2(\mathbb{R}^2) \), will have surface states with a non-zero density on an appropriate scale, for suitable \( t \in (0, 1) \). To distinguish the bulk from the surface density of states for this problem, we consider the operators \(-\Delta + W_t \) on squares \( Q_n = (-n, n)^2 \) with Dirichlet boundary conditions, for \( n \) large, count the number of eigenvalues inside a compact subset of a non-degenerate spectral gap of \( D_0 \) and scale with \( n^{-2} \) for the bulk and with \( n^{-1} \) for the surface states. Taking the limits \( n \to \infty \) (which exist as explained in [DS, EKSchrS]), we obtain the integrated density of states measures \( \rho_{\text{bulk}}(D_t, I) \) for the bulk and \( \rho_{\text{surf}}(D_t, J) \) for the surface states of this model; here \( I \subset \mathbb{R} \) and \( J \subset \mathbb{R} \setminus \sigma(D_0) \) are open intervals and \( \mathcal{T} \subset \mathbb{R} \setminus \sigma(D_0) \).
Our main result can be described as follows: If \((a, b)\) is a (non-trivial) spectral gap of the periodic operator \(-\Delta + V\), acting in \(L_2(\mathbb{R}^2)\), then for any compact interval \([\alpha, \beta] \subset (a, b)\) with \(\alpha < \beta\) there is a \(t \in (0, 1)\) such that \(\rho_{\text{surf}}(D_t, (\alpha, \beta)) > 0\). Upper bounds for the surface density of states are discussed in [HK].

Our paper is organized as follows. Section 2 deals with dislocation on the real line. Here it is shown that the \(k\)-th gap in the essential spectrum of \(H_t\) (if it is open) is crossed by effectively \(k\) eigenvalues of \(H_t\) as \(t\) increases from 0 to 1. As an example, we discuss a periodic step potential in Section 3 where one can compute the eigenvalues of the dislocation operator numerically. Note that our calculations yield numbers which are exact up to finding the zeros of some transcendental functions. Related pictures can be found in [DPR] where a different numerical approach has been used.

In Section 4 we adapt the method of Section 2 to the dislocation problem on the strip \(\Sigma\). The results obtained for the strip then easily yield spectral information for the dislocation problem in the plane. Section 5 presents examples from the class of muffin tin potentials where one can “see” the motion of the eigenvalues rather directly for either translation in the \(x\)-direction or in the \(y\)-direction. Finally, we include an Appendix on regularity properties of the functions describing the eigenvalues of the dislocation operator \(H_t\) in one dimension.

For basic notation and definitions concerning self-adjoint operators in Hilbert space, we refer to [K, RS-I].

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2. Dislocation on the real line

In this section, we study perturbations of periodic Schrödinger operators on the real line where the potential is obtained from a periodic potential by a coordinate shift on the left half-axis.

Let \(h_0\) denote the (unique) self-adjoint extension of \(-\frac{d^2}{dx^2}\) defined on \(C_0^\infty(\mathbb{R})\). Our basic class of potentials is given by

\[ P := \{ V \in L_{1,\text{loc}}(\mathbb{R}, \mathbb{R}) ; \forall x \in \mathbb{R} : V(x + 1) = V(x) \} . \]  

(2.1)

Potentials \(V \in P\) belong to the class \(L_{1,\text{loc,unif}}(\mathbb{R})\) which coincides with the Kato-class on the real line; in particular, any \(V \in P\) has relative form-bound zero with respect to \(h_0\) and thus the form-sum \(H\) of \(h_0\) and \(V \in P\) is well defined (cf. [CFrKS]). For \(V \in P\) given, we define the dislocation potentials \(W_t\) as in eqn. (1.1), for \(0 \leq t \leq 1\); as before, the form-sum \(H_t\) of \(h_0\) and \(W_t\) is well defined.

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

\[ \sigma(H) = \sigma_{\text{ess}}(H) = \bigcup_{k=1}^\infty [\gamma_k, \gamma'_k] , \]  

(2.2)
where the $\gamma_k$ and $\gamma_k'$ 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

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

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

In addition to the essential spectrum, the operators $H_t$ may have discrete eigenvalues below the infimum of the essential spectrum and inside any (non-degenerate) gap, for $t \in (0, 1)$; these eigenvalues are simple. The eigenvalues of $H_t$ in the gaps of $H$ depend continuously on $t$; cf. the Appendix for a brief exposition of the relevant perturbational arguments, which are fairly standard. A more complete and precise picture is established in the following lemma which says that the discrete eigenvalues of $H_t$ inside a given gap $\Gamma_k$ of $H$ can be described by an (at most) countable, locally finite family of continuous functions, defined on suitable subintervals of $[0, 1]$.

**Lemma 2.1.** Let $k \in \mathbb{N}$ and suppose that the gap $\Gamma_k$ of $H$ is open, i.e., $\gamma_k' < \gamma_{k+1}$. Then there is a (finite or countable) family of continuous functions $f_j: (\alpha_j, \beta_j) \to \Gamma_k$, where $0 \leq \alpha_j < \beta_j \leq 1$, 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 $[a', b'] \subset \Gamma_k$.

For the convenience of the reader, we include a proof in the Appendix. Under stronger assumptions on $V$ one can show that the eigenvalue branches are H"older- or Lipschitz-continuous, or even analytic; cf. the Appendix. Additional information on the eigenvalue functions $f_j$ can be found in [K1, K2].

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 2.1 and writing $f_i(\alpha_i) := \lim_{t \downarrow \alpha_i} f_i(t)$,
Proof. We may assume that the eigenvalues of
where
σ

min-max. Since the Hilbert space
Now the usual perturbational and variational arguments for qua-

dratic forms (K) allow us to consider a sequence of approximations on intervals
operators, we recommend [P, Saf]. In this section lies in testing our approach in the simplest possible case. For further
higher dimensions, as will be seen in the sequel. In this sense, the importance of
other hand, our variational arguments are more flexible and allow an extension to
(a eigenvalue and a resonance) in any given gap of the periodic problem. On the
side, we show that the eigenvalues of the
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 ∈ Γ
k as t goes from 0 to 1. To obtain
the result of Theorem 2.2 we only have to take the limit
n → ∞. 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 2.3. The eigenvalues of
H
n,t depend continuously on t ∈ [0, 1].

Proof. We may assume that the eigenvalues of
H
n,t are numbered according to
min-max. Since the Hilbert space
L
2(−n − t, n) depends on t, we use the unitary mappings

U
n,t : L
2(−n − t, n) → L
2(−n, n),

(U
n,t f)(x) := \sqrt{\sigma_n t} f(\sigma_n x),

where
\sigma_n := \frac{2n + t}{2n}. Let
\tilde{H}_n,t := U_{n,1} H_n,t U_{n,1}^{-1}
and
\tilde{W}_t(x) := W_1(\sigma_n x) so that
(writing \sigma = \sigma_n)

\tilde{H}_n,t = \sigma^{-2} h_0 + \tilde{W}_t(x) = \sigma^{-2} (h_0 + \sigma^2 \tilde{W}_t(x)).

It is easy to see that the mapping
[0, 1] \ni t \mapsto \sigma^2 \tilde{W}_t ∈ L
1(−n, n) is continuous.
Now the usual perturbational and variational arguments for quadratic forms ([K]
and the Appendix) imply that the eigenvalues of \( h_0 + \sigma^2 \hat{W}_t \) depend continuously on \( t \), and then the same is true for the eigenvalues of \( H_{n,t} \).

The next lemma is to establish a connection between the spectra of \( H_t \) and \( H_{n,t} \) for \( 0 \leq t \leq 1 \) and \( n \) large. In the proof and henceforth, we will make use of the following cut-off functions: We pick some \( \varphi \in C_c^\infty(-2,2) \) with \( 0 \leq \varphi \leq 1 \) and \( \varphi(x) = 1 \) for \( |x| \leq 1 \). For \( k \in (0,\infty) \) we then define \( \varphi_k(x) := \varphi(x/k) \) so that \( \text{supp } \varphi_k \subset (-2k,2k) \), \( \varphi_k(x) = 1 \) for \( |x| \leq k \), \( |\varphi'_k(x)| \leq Ck^{-1} \) and \( |\varphi''_k(x)| \leq Ck^{-2} \).

Finally, we let \( \psi_k := 1 - \varphi_k \). For any self-adjoint operator \( T \) we denote the spectral projection associated with an interval \( I \subset \mathbb{R} \) by \( P_I(T) \) and we write \( \dim P_I(T) \) to denote the dimension of the range of the projection \( P_I(T) \).

**Lemma 2.4.** 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 \( n \geq n_0 \), and

\[
\dim P_{(\eta_1, \eta_2)}(H_t) = \dim P_{(\eta_1, \eta_2)}(H_{n,t}), \quad n \geq n_0. \tag{2.7}
\]

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

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

\[
|H_{n,t}u_k - Eu_k| \leq 2 \|\varphi'_k\|_\infty \|u\| + |\varphi''_k|_\infty \|u\|, \tag{2.8}
\]

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

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

\[
v_{1,n_j} := \varphi_{k_j} u_{n_j,t}, \quad v_{2,n_j} := \psi_{k_j} u_{n_j,t}, \tag{2.9}
\]

so that \( v_{1,n_j} \in D(H_t) \) and \( \|(H_t - \eta)v_{1,n_j}\| \to 0 \) as \( j \to \infty \) by a similar estimate as in part (1) (and using a simple bound for \( \|u_{n_j,t}\| \) 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 \( \|v_{1,n_j}\| \to 1 \)) as \( j \to \infty \): The function

\[
v_{2,n_j} := \begin{cases} v_{2,n_j}(x), & x \geq 0, \\ v_{2,n_j}(x - t), & x < 0, \end{cases} \tag{2.10}
\]

belongs to the domain of \( H_{n_j,0} \) and \( H_{n_j,0}v_{2,n_j} = [H_{n_j,0}v_{2,n_j}]^- \), where \([x]^=\) is defined in analogy with eqn. \( (2.10) \). Since we also have \( (H_{n_j,t} - \eta)v_{2,n_j} \to 0 \), as \( j \to \infty \), we see that \( (H_{n_j,0} - \eta)v_{2,n_j} \to 0 \). But dist(\( \eta, \sigma(H_{n,0}) \)) \( \geq \delta_0 > 0 \) for all \( n \) and the Spectral Theorem implies that \( \|v_{2,n_j}\| \to 0 \) as \( j \to \infty \). We have thus shown that \( \|v_{1,n_j}\| \to 1 \) and \( \|(H_t - \eta)v_{1,n_j}\| \to 0 \) which implies that \( \eta \in \sigma(H_t) \).

3. It remains to show that \( \dim P_{(\eta_1, \eta_2)}(H_{n,t}) \leq \dim P_{(\eta_1, \eta_2)}(H_t) \), for \( n \) large. The proof by contradiction follows the lines of part (2); instead of a sequence of functions \( u_{n_j} \), we work with an orthonormal system \( u_{n_j}^{(1)}, \ldots, u_{n_j}^{(\ell)} \) of eigenfunctions where \( \ell = \dim P_{(\eta_1, \eta_2)}(H_t + 1) \). We leave the details to the reader. \( \square \)
Remark 2.5. 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 $\Gamma_k$ 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 $(E - ce^{-\alpha n}, E + ce^{-\alpha n})$, for $n$ large. There is a similar converse statement with the roles of $H_t$ and $H_{n,t}$ exchanged; cf. also Remark 4.2 for further discussion.

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 2.4 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 2.6. 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

$$E_j \notin \sigma(H_t) \cup \sigma(H_{n,t}), \quad \forall t \in [t_{j-1}, t_j], \quad j = 1, \ldots, K, \quad n \geq n_0. \quad (2.11)$$

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 $\eta_t \notin \sigma(H_t)$ for all $t \in (t - \varepsilon_t, t + \varepsilon_t)$. 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 $E_j := \eta_{\tau_j}$. 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 2.4, using Lemma 2.3 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 2.2.

Proof of Theorem 2.2. Let $E_j$ be as in Lemma 2.6 and $N_k$ as in eqn. (2.4). We fix some $E \in \Gamma_k$ such that $E > E_j$ for $j = 0, \ldots, K$ and $E \notin \sigma(H_t) \cup \sigma(H_{n,t})$ for $j = 0, \ldots, K$ and for all $n$ large. It is then easy to see that

$$N_k = \sum_{j=1}^{K} \left( \dim P_{(E_j, E)}(H_{t_j}) - \dim P_{(E_j, E)}(H_{t_j-1}) \right) \quad (2.12)$$

and that

$$\dim P_{(-\infty, E]}(H_{n,1}) - \dim P_{(-\infty, E]}(H_{n,0})$$

$$= \sum_{j=1}^{K} \left( \dim P_{(E_j, E)}(H_{n,t_j}) - \dim P_{(E_j, E)}(H_{n,t_j-1}) \right). \quad (2.13)$$

The LHS of (2.13) equation equals $k$. Furthermore, by Lemma 2.4, we have

$$\dim P_{(E_j, E)}(H_{t_j}) = \dim P_{(E_j, E)}(H_{n,t_j}) \quad (2.14)$$

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


3. A one-dimensional periodic step potential

In this section, we study the one-dimensional $2\pi$-periodic potential

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

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

\[ D(E) := \varphi_1(2\pi; E) + \varphi_2(2\pi; E) = \begin{vmatrix} \varphi_1(2\pi; E) & \varphi'_1(2\pi; E) \\
\varphi_2(2\pi; E) & \varphi'_2(2\pi; E) \end{vmatrix} \]  

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

\[ -u'' + (V - E)u = 0 \]  

and satisfy the boundary conditions

\[ \varphi_1(0; E) = \varphi'_2(0; E) = 1 \quad \text{and} \quad \varphi'_1(0; E) = \varphi_2(0; E) = 0. \]  

The matrix $M(E)$ on the RHS of (3.2) is called the monodromy matrix. A simple computation shows that $[-1/2, 1/2] \subset \Gamma_1$, where $\Gamma_1$ is the first spectral gap of $H$ (with numbering according to Floquet theory). Note that the gap edges of $\Gamma_1$ also equal the first eigenvalue in the (semi-)periodic eigenvalue problem for $-\frac{d^2}{dx^2} + V$ 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 (3.3); 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 potentials $W_t$ 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.,

\[ \varphi_-(t; E) = \varphi_+(0; E) \quad \text{and} \quad \varphi'_-(t; E) = \varphi'_+(0; E). \]  

An equivalent condition for (3.5) is the equality of the ratio functions $\frac{\varphi_-(t; E)}{\varphi'_-(t; E)}$ and $\frac{\varphi_+(0; E)}{\varphi'_+(0; E)}$, cf. [DPR]. We compute the Floquet solutions $\varphi_{\pm}$ 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, we divide $[-1/2, 1/2]$ into 100 subintervals of equal length and compute numerical values for $t$ such that

\[ \left| \frac{\varphi_-(t; E)}{\varphi'_-(t; E)} - \frac{\varphi_+(0; E)}{\varphi'_+(0; E)} \right| < \varepsilon, \]  

where the error $\varepsilon > 0$ is small. This leads to the following plot of $t \mapsto E(t)$, see Fig. 1.
4. 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 $W_t$ defined as in eqn. (1.2); again, the parameter $t$ ranges between 0 and 1. 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., $\sigma_{\text{ess}}(S_t) = \sigma_{\text{ess}}(S_0)$ for all $t \in [0,1]$. As in Section 2, 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.)

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 4.1.** 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 $\Sigma$. Let

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

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 $E \in \sigma_{\text{disc}}(S_{n,t_n})$; 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 $\varphi_n$ as in Section 2 and denote the natural extension to $\mathbb{R}^2$ again by $\varphi_n$. We let $\psi_n = 1 - \varphi_n$. Clearly,

$$\|(S_{t_n} - E)(\varphi_{n/4} u_n)\|, \|(S_{n,t_n} - E)(\psi_{n/4} u_n)\| \leq c/n, \quad (4.2)$$

for some $c \geq 0$. There is a subsequence $(t_{n_j})_{j \in \mathbb{N}} \subset (t_n)_{n \in \mathbb{N}}$ and $\mathcal{T} \in [0, 1]$ s.th. $t_{n_j} \to \mathcal{T}$ as $j \to \infty$. Since $V$ is Lipschitz, we may infer from (4.2) that

$$\|(S_{\mathcal{T}} - E)(\varphi_{n/4} u_{n_j})\| \to 0, \quad j \to \infty, \quad (4.3)$$

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

$$\bar{v}(x, y) := \begin{cases} v(x, y), & x > 0, \\ v(x - t, y), & x < 0, \end{cases} \quad (4.4)$$

in analogy with eqn. (2.10). Then $[\psi_{n/4} u_n]^- \in D(S_{n,0})$ and

$$\|(S_{n,0} - E)[\psi_{n/4} u_n]^-\| = \|(S_{n,t_n} - E)(\psi_{n/4} u_n)\| \leq c/n. \quad (4.5)$$

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 $[\psi_{n/4} u_n]^- \to 0$ (and therefore also $\psi_{n/4} u_n \to 0$) as $n \to \infty$.

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

**Remark 4.2.** By a well-known line of argument, one can obtain *exponential localization* of the eigenfunctions of $S_1$ near the interface \{(x, y) | x = 0\}. Since we will use exponential localization in a more systematic way in the forthcoming paper [HK] we only give a brief sketch here: Suppose that $E \in (a, b)$ and $t \in (0, 1)$ satisfy $E \in \sigma(S_1)$. Let $u \in D(S_0) = D(S_t)$ denote a normalized eigenfunction and let $\varphi_n$, $n \in \mathbb{N}$, be as in the proof of Theorem 4.1. As above, we have

$$(S_t - E)(\varphi_n u) = -2\nabla \varphi_n \cdot \nabla u - (\Delta \varphi_n) u =: r_n, \quad (4.6)$$

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

$$\|\chi_{|x| \geq 4n} u\| \leq \|\chi_{|x| \geq 4n}(S_t - E)^{-1} r_n\| \leq C e^{-\alpha n}, \quad (4.7)$$

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

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

$$D_t = -\Delta + W_t, \quad 0 \leq t \leq 1. \quad (4.8)$$
Denote by $S_t(\theta)$ the operator $S_t$ with $\theta$-periodic boundary conditions in the $y$-variable. Since $W_t$ is periodic with respect to $y$, we have

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

and hence the spectrum of $D_t$ has a band-gap structure; furthermore, $D_t$ has no singular continuous part, cf. [DS, FS]. As for the spectrum of $S_t$ inside the gaps of $S_0$, Theorem 4.1 leads to the following result.

**Theorem 4.3.** Let $(a, b)$ denote a spectral gap of $D_0$, $a > \inf \sigma_{\text{ess}}(D_0)$, 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 4.1 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

$$(D_t - E)(\Phi_n \tilde{u}_n) = (-\partial_x^2 - \partial_y^2 + W_t - E)(\varphi_n(x)\varphi_n(y)\tilde{u}_n(x, y))$$

$$= \varphi_n(y)[(S_t - E)(\varphi_n(x) u_n)]' - \varphi_n(x)(2\varphi'_n(y)\partial_y \tilde{u}_n + \varphi_n''(y)\tilde{u}_n).$$

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

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

while $||\Phi_n \tilde{u}_n|| \geq c_0n$ with a constant $c_0 > 0$. This implies the desired result.  \[ \square \]

**Remark 4.4.** We learn from the above proof that there are functions

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

(4.12)

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

$$(D_t - E)v_n \to 0, \quad n \to \infty.$$  (4.13)

These functions play a key role in our analysis of the rotation problem at small angle in [HK].

We finally turn to a brief discussion of the i.d.s. (the integrated density of states [V]) for the dislocation operators $D_t$. We adopt the natural distinction of [DS, EKSchrS, KS] 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 $\overline{J} \subset \mathbb{R} \setminus \sigma(D_0)$

$$\rho_{\text{bulk}}(I, D_t) = \lim_{n \to \infty} \frac{1}{4n^2} N(I, D_t^{(n)}), \quad \rho_{\text{surf}}(J, D_t) = \lim_{n \to \infty} \frac{1}{2n} N(J, D_t^{(n)}).$$  (4.14)
The existence of the limits in (4.14) 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 eqn. (4.14) 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 $\rho_{\text{surf}}$ 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 4.5.** 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 4.3 and Remark 4.4 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, $\nu$ corresponds to the $n$ of Remark 4.4. We then see that the functions $\varphi_k$, 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 $M_n := \text{span}\{\varphi_k \mid k \in \mathbb{N}, k \leq \frac{1}{2}(\frac{n}{\nu} - 1)\}$, it is clear that dim $M_n \geq n/(3\nu)$, 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 $(\alpha, \beta)$; we will show that dim $\mathcal{N}_n \geq \text{dim} M_n$ which implies the desired result. If we assume for a contradiction that dim $\mathcal{N}_n < \text{dim} M_n$ 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, $\|(D_t(n) - E)v\| \geq \varepsilon$. On the other hand, $v$ is a finite linear combination of the $\varphi_k$, which implies $\|(D_t(n) - E)v\| < \varepsilon$. \hfill \Box

We will continue the discussion of bulk versus surface states in the companion paper [HK] where a corresponding upper bound of the form $N(J, D_t(n)) \leq cn \log n$ is provided.

### 5. 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

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

and we let $V = V_{r, P_0}$ be zero on $\Omega_{r, P_0}$ 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 4. 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 $\{(x, y) \mid x = 0\}$. Defining the dislocation potential $W_t$ as in Section 4, we see that there are bulk states given by the Dirichlet eigenvalues of the disc of radius $r$; 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 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 $\lambda_k = \mu_k(r)$ 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 $\lambda_k$ as $t \uparrow 1/2 + r$ and to $+\infty$ as $t \downarrow 1/2 - r$. In this simple model, the eigenvalues $\mu_k$ 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 4 (Corollary 4.5).

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. In [HK] we will again use muffin tin potentials as examples for the rotation problem. In that paper, we will also discuss approximations by muffin tin potentials of height $n$ and their limit as $n \to \infty$.

(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 the half-discs on the right are not shifted by $t$ in the y-direction. The surface states correspond to the states of the Dirichlet Laplacian on the union $\Omega_{t, r, \text{surf}}$ of these half-discs. There are two cases: either $\Omega_{t, r, \text{surf}}$ is connected and we have a scattering channel along the interface, or $\Omega_{t, r, \text{surf}}$ is the disjoint union of a sequence of bounded domains; cf. Figure 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 $\Omega_{t, r, \text{surf}}$ are disconnected for $0 \leq t \leq \tau_0$ and for $\tau_1 \leq t \leq 1$; for $\tau_0 < t < \tau_1$, however, $\Omega_{t, r, \text{surf}}$ is connected and forms a periodic wave guide with purely a.c. spectrum [SW]; cf. also [DS]. 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.

\[ \text{Figure 2: Muffin tins: two cases for dislocation in the } y \text{-direction.} \]

Note that, if we had chosen \( x_0 = \frac{1}{2} \), then nothing at all would have happened for translation in the \( y \)-direction.

(The authors thank A. Ruschhaupt, Hannover, for asking about translation in the \( y \)-direction.)

6. Appendix: Continuity and Regularity of Eigenvalues

In this appendix, we discuss several basic facts concerning continuity and regularity of the eigenvalue branches for the one-dimensional dislocation problem. We first consider potentials \( V \) from the class \( P \subset L^1_{\text{loc,unif}}(\mathbb{R}) \) as in (2.1) where the eigenvalues are continuous functions of the dislocation parameter \( t \). In the subsequent estimates we will use

\[ |V|_{1, \text{loc,unif}} := \sup_{y \in \mathbb{R}} \int_y^{y+1} |V(x)| \, dx \quad (A.1) \]

as a natural norm on \( L^1_{\text{loc,unif}}(\mathbb{R}) \). As is well known (cf., e.g., [CFrKS]), any potential \( V \in L^1_{\text{loc,unif}}(\mathbb{R}) \) is relatively form-bounded with respect to \( h_0 \) with relative form-bound zero. More precisely, we have the following lemma.

**A.1. Lemma.** For any \( \varepsilon > 0 \) there exists a constant \( C_\varepsilon \geq 0 \) such that for any \( V \in L^1_{\text{loc,unif}}(\mathbb{R}) \) we have

\[ \int_{\mathbb{R}} |V| |\varphi|^2 \, dx \leq |V|_{1, \text{loc,unif}} \left( \varepsilon |\varphi'|^2 + C_\varepsilon |\varphi|^2 \right), \quad \varphi \in H^1(\mathbb{R}). \quad (A.2) \]

**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: \( \text{supp } \zeta_1 \subset (0, \varepsilon) \), each \( \zeta_n \) is a translate of \( \zeta_1 \), \( M := \sup_{x \in \mathbb{R}} \sum_{n \in \mathbb{N}} |\zeta_n'(x)|^2 \) is finite and \( \sum_{n \in \mathbb{N}} \zeta_n^2(x) = 1 \) for all \( x \in \mathbb{R} \). By the IMS localization formula (see [CFrKS]), we have for any \( \varphi \in C_c^\infty(\mathbb{R}) \),

\[ |\varphi'|^2 = (\varphi'', \varphi) = \sum_{n=1}^\infty |(\zeta_n \varphi)'|^2 - \sum_{n=1}^\infty |\zeta_n' \varphi|^2 \geq \sum_{n=1}^\infty |(\zeta_n \varphi)'|^2 - M \| \varphi \|^2, \]
so that

\[
\int |V(x)||\varphi(x)|^2 \, dx \leq \sum_{n=1}^{\infty} |\zeta_n|^2 \int_{\text{supp } \zeta_n} |V(x)| \, dx \\
\leq \varepsilon \left(|\varphi'|^2 + M |\varphi|^2\right) |V|_{1,\text{loc,unif}}.
\]

The general case follows by approximation and Fatou’s lemma. \(\square\)

For \(V \in P\), the function

\[
\vartheta_V(s) := \int_0^s |V(x + s) - V(x)| \, dx, \quad 0 \leq s \leq 1,
\]

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

**A.2. Lemma.** Let \(V \in P\), \(E_0 \in \mathbb{R} \setminus \sigma(H_{t_0})\), and write \(\varepsilon_0 := \text{dist}(E_0, \sigma(H_{t_0}))\). 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 \(\tau_1 \in (0, \tau_0)\)

\[
\|(H_t - E_0)^{-1} - (H_{t_0} - E_0)^{-1}\| \leq C \vartheta_V(t - t_0), \quad |t - t_0| < \tau_1.
\]

**Proof.** Without loss of generality we may assume that \(V \geq 1\). Let \(h_t\) denote the quadratic form associated with \(H_t\). Applying Lemma A.1 (with \(\varepsilon := 1\)) we see that

\[
|h_t[u] - h_{t_0}[u]| \leq \int_{\mathbb{R}} |W_t - W_{t_0}| |u|^2 \, dx \leq C_1 \vartheta_V(t - t_0) h_{t_0}[u], \quad u \in H^1(\mathbb{R}),
\]

with some constant \(C_1\). The desired result now follows by [K; Thm. VI-3.9]. \(\square\)

We therefore see that \(H_{t_n} \to H_{t_0}\) in the sense of norm resolvent convergence if \(t_n \in [0, 1], (t_n)_{n \in \mathbb{N}} \subset [0, 1]\) and \(t_n \to t_0\). By standard arguments, this implies that the discrete eigenvalues of \(H_t\) depend continuously on \(t\). We are now prepared for the proof of Lemma 2.1.

**Proof of Lemma 2.1.** We consider \(t \in T\), the flat one-dimensional torus, and we denote the spectral gap by \((a, b)\). Let \([a', b'] \subset (a, b)\).

1. Let \((\eta, \tau) \in (a, b) \times T\). Since \(\sigma(H_T) \cap (a, b)\) is a discrete set, and since \(\sigma(H_t)\) depends continuously on \(t\), there is a neighborhood \(U_{\eta, \tau} \subset (a, b) \times T\) of \((\eta, \tau)\) 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 \(\sigma(H_t) \cap (\eta_1, \eta_2) = \emptyset\),

or

**Type (2):** \(\eta\) is an eigenvalue of \(H_T\) and there is a continuous function \(f: (\tau_1, \tau_2) \to (\eta_1, \eta_2)\) such that \(f(t)\) is an eigenvalue of \(H_t\); \(H_t\) has no further eigenvalues in \((\eta_1, \eta_2)\), for \(\tau_1 < t < \tau_2\).

Now the family \(\{U_{\eta, \tau} : (\eta, \tau) \in (a, b) \times T\}\) is an open cover of \((a, b) \times T\) and there exists a finite selection \(\{U_{\eta, \tau} \}_{i=1}^N\) such that

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

(2) Suppose that $(\eta, \tau) \in (a, b) \times \mathbb{T}$ is such that $\eta \in \sigma(H_{\tau})$ and let $f : (\tau_1, \tau_2) \rightarrow (\eta_1, \eta_2)$ as above. Consider a sequence $(t_j)_{j \in \mathbb{N}} \subset (\tau_1, \tau_2)$ with $t_j \rightarrow \tau_1$. We can find a subsequence $(t_{j_k})_{k \in \mathbb{N}}$ such that $f(t_{j_k}) \rightarrow \bar{\eta}$ 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 $\tau_1$. It follows that there exist a maximal open interval $(\alpha, \beta) \subset (0, 1)$ and a (unique) continuous extension $\tilde{f} : (\alpha, \beta) \rightarrow (a, b)$ 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 $t_j \rightarrow \alpha$ has a subsequence $(t_{j_k})_{k \in \mathbb{N}}$ such that $\tilde{f}(t_{j_k}) \rightarrow \bar{\eta}$ 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 $\alpha$, contradicting the maximality property of the interval $(\alpha, \beta)$.

Suppose there are sequences $(t_j)_{j \in \mathbb{N}}, (s_j)_{j \in \mathbb{N}} \subset (\alpha, \beta)$ such that $t_j \rightarrow \alpha$ and $s_j \rightarrow \alpha$ and $\tilde{f}(t_j) \rightarrow \alpha$ while $\tilde{f}(s_j) \rightarrow b$ as $j \rightarrow \infty$. Then for any $\eta' \in (a, b)$ there is a sequence $(r_j)_{j \in \mathbb{N}} \subset (\alpha, \beta)$ such that $r_j \rightarrow \alpha$ and $\tilde{f}(r_j) \rightarrow \eta'$, 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 2.1. With $\vartheta_V : [0, 1] \rightarrow [0, \infty)$ as in (A.3), we study potentials from the classes

$$\mathcal{P}_\alpha := \{ V \in \mathcal{P} \mid \exists C \geq 0 : \vartheta_V(s) \leq Cs^\alpha, \forall 0 < s \leq 1 \}, \quad (A.5)$$

where $0 < \alpha \leq 1$. The class $\mathcal{P}_\alpha$ consists of all periodic functions $V \in \mathcal{P}$ which are (locally) $\alpha$-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. It will be shown below that $\mathcal{P}_1$ coincides with the class of periodic functions on the real line which are locally of bounded variation. We first prove Lipschitz-continuity of the eigenvalues of $H_t$ for $V \in \mathcal{P}_1$.

**A.3. Proposition.** For $V \in \mathcal{P}_1$, let $(a, b)$ denote any of the gaps $\Gamma_k$ of $H$ and let $f_j : (\alpha_j, \beta_j) \rightarrow (a, b)$ be as in Lemma 2.1. Then the functions $f_j$ are uniformly Lipschitz-continuous. More precisely, for each gap $\Gamma_k$ there exists a constant $C_k \geq 0$ such that for all $j$

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

**Proof.** As in the proof of Lemma 2.6 we can find a finite number of levels $E_1, \ldots, E_\ell \in (a, b)$ and a partition $0 = \tau_0 < \tau_1 < \ldots < \tau_{\ell - 1} < \tau_\ell = 1$ such that $E_j \notin \sigma(H_t)$ for all $t \in I_j := [\tau_{j-1}, \tau_j]$ and for $j = 1, \ldots, \ell$. Now $V \in \mathcal{P}_1$ implies $|W_t - W_{t'}|_{1, \text{loc}, \text{unif}} = \vartheta_V(t - t') \leq C|t - t'|$ and we conclude with the aid of Lemma A.2 that there are constants $c_1, \ldots, c_\ell \geq 0$ such that

$$\|(H_t - E_j)^{-1} - (H_{t'} - E_j)^{-1}\| \leq c_j|t - t'|, \quad t, t' \in I_j.$$
This implies that the min-max-values $\mu_k(s)$ of $(H_s - E_j)^{-1}$ satisfy

$$|\mu_k(t) - \mu_k(t')| \leq c_j |t - t'|, \quad t, t' \in I_j.$$ 

By the spectral mapping theorem, the eigenvalues of $H_t$ in $(E_j, b)$ are in bijection with the eigenvalues of $(H_t - E_j)^{-1}$ in $(\frac{1}{b-E_j}, \infty)$. We now let $C := \max\{c_1, \ldots, c_\ell\}$ to finish our proof. □

A.4. Remarks.
(a) By the same argument, we obtain the following result on Hölder-continuity: If $0 < \alpha < 1$ and $V \in P_\alpha$, then each of the functions $f_j: (\alpha_j, \beta_j) \to (a, b)$ 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 $(\alpha_j, \beta_j)$, much less a constant that would be uniform for all $j$.

(b) For analytic potentials $V$, it is shown in [K1] that the eigenvalue branches $f_j$ in Lemma 2.1 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 $W^1_2$-functions near the gap edges if the potential is in $L^2(T)$.

We finally give a characterization of the class $P_1$.

A.5. Proposition. Let $BV_{\text{loc}}(\mathbb{R})$ denote the space of real-valued functions which are of bounded variation over any compact subset of the real line.

Then $P_1 = P \cap BV_{\text{loc}}(\mathbb{R})$.

It is easy to see that any $V \in P \cap BV_{\text{loc}}(\mathbb{R})$ belongs to $P_1$: certainly, any $V \in P$ which is monotonic over $[0, 1]$ is an element of $P_1$ and any function of bounded variation can be written as the difference of two monotonic functions.

The converse direction is established by the following result due to J. Voigt, Dresden; cf. also [EG, Chapter 5] for related material on $BV$-functions of several variables.

A.6. Lemma. Let $f \in L^1_{\text{loc}}(\mathbb{R}, \mathbb{R})$ be periodic with period 1 and suppose that there are $c \geq 0$, $\varepsilon > 0$ such that

$$\int_0^1 |f(x + t) - f(x)| \, dx \leq ct, \quad \forall 0 < t < \varepsilon. \quad (A.6)$$

Consider $f$ as a function in $L^1(\mathbb{T})$, with $\mathbb{T}$ denoting the one-dimensional torus.

We then have: the distributional derivative $\Delta f$ is a (signed) Borel-measure $\mu$ 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 $\eta: C^1(T) \to \mathbb{R}$ by

$$\eta(\varphi) := -\int_0^1 \varphi' f \, dx,$$

we may compute

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

$$= \lim_{t \to 0} \int_0^1 \varphi(x) \frac{1}{t} (f(x+t) - f(x)) \, dx,$$

and the assumption (A.6) yields the estimate $|\eta(\varphi)| \leq c \|\varphi\|_\infty$. Since $C^1(T)$ is dense in $C(T)$, the functional $\eta$ has a unique continuous extension to all of $C(T)$; we denote the extension by the same symbol $\eta$. By the Riesz representation theorem there is a measure $\mu$ such that $\eta(\varphi) = \int \varphi \, d\mu$ for all $\varphi \in C(T)$. Furthermore, for $\varphi \in C^1(T)$ we have $-\int_0^1 \varphi' f \, dx = \int_0^1 \varphi \, d\mu$, and we see that $\mu = \partial f$ on $T$ in the distributional sense. The choice $\varphi := 1$ yields $\int_T d\mu = -\int_0^1 \varphi' f \, dx = 0$ and the function $\tilde{f}(x) := \mu([0, x))$ satisfies $\partial \tilde{f} = \mu$. This is easy to check: for $\varphi \in C^1(T)$ we have

$$\int \tilde{f} \varphi' \, dx = \int_0^1 \int_{0 \leq y < x} d\mu(y) \varphi'(x) \, dx$$

$$= \int_{0 \leq y < 1} \int_0^1 \varphi'(x) \, dx \, d\mu(y) = -\int_{[0,1]} \varphi(y) \, d\mu(y).$$

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

References

[ADH] S Alama, PA Deift, and R Hempel, Eigenvalue branches of the Schrödinger operator $H - \lambda W$ in a gap of $\sigma(H)$, Commun. Math. Phys. 121 (1989), 291–321

[AM] NW Ashcroft and ND Mermin, Solid State Physics, Holt, Rinehart and Winston, New York, 1976

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

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

[DH] PA Deift and R Hempel, On the existence of eigenvalues of the Schrödinger operator $H - \lambda W$ in a gap of $\sigma(H)$, Commun. Math. Phys. 103 (1986), 461–490

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

[DPR] T Dohnal, M Plum, and W Reichel, Localized modes of the linear periodic Schrödinger operator with a nonlocal perturbation, http://digbib.ubka.uni-karlsruhe.de/volltexte/1000009828 (Preprint 2008)

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

[EG] LC Evans and RF Gariepy, Measure Theory and Fine Properties of Functions, CRC Press (1992)

[EKSchrS] H Englisch, W Kirsch, M Schröder, and B Simon, Random Hamiltonians ergodic in all but one direction, Commun. Math. Phys. 128 (1990), 613–625
N. Filonov and A. Sobolev, *Absence of the singular continuous component in the spectrum of analytic direct integrals*, Zapiski Nauchnykh Seminarov POMI 318 (2004) 298–307

D. Gilbarg and N.S. Trudinger, *Elliptic Partial Differential Equations of Second Order*, Springer, New York, 1977

R. Hempel and M. Kohlmann, *Spectral properties of grain boundaries at small angle of rotation*, to appear in: J. Spectral Theory

T. Kato, *Perturbation Theory for Linear Operators*, Springer, New York, 1966

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

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

A. Pushnitski, *Operator theoretic methods for the eigenvalue counting function in spectral gaps*, Ann. Henri Poincaré 10 (2009), 793–822

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

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

O. Safronov, *The amount of discrete spectrum of a perturbed periodic Schrödinger operator inside a fixed interval* $(\lambda_1, \lambda_2)$, Int. Math. Res. Notices (2004), 411–423

A. Sobolev and J. Walthoe, *Absolute continuity in periodic wave guides*, Proc. Lond. Math. Soc. 85, no 3, (2002), 717–741

I. Veselic, *Existence and regularity properties of the integrated density of states of random Schrödinger operators*, Springer Lecture Notes in Mathematics, vol. 1917, Springer, New York, 2008

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