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A variational approach to dislocation problems for periodic Schrödinger operators

Rainer Hempel [a], Martin Kohlmann [b,*]

[a] Institute for Computational Mathematics, Technische Universität Braunschweig, Pockelsstraße 14, 38106 Braunschweig, Germany
[b] Institute for Applied Mathematics, Leibniz Universität Hannover, Welfengarten 1, 30167 Hannover, Germany

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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 $x \geqslant 0$, 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 (Korotyaev (2000, 2005) [15,16]) on the real line. We then proceed to the dislocation problem for an infinite strip and for the plane. In Appendix A, 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. [2], 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. [6]: 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 $\{x \in \mathbb{R}^d \mid x_1 \geqslant 0\}$ 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 [13] we will then study some aspects of the *rotation problem* where we take the given periodic potential V in the right half-plane and a rotated version $V \circ M_\vartheta$ in the left half-plane with M_ϑ denoting rotation by the angle ϑ; some results from the present paper will be essential for [13].

* Corresponding author.
E-mail addresses: r.hempel@tu-bs.de (R. Hempel), kohlmann@ifam.uni-hannover.de (M. Kohlmann).

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

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

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 $0 \leqslant t \leqslant 1$; also H_t cannot have any embedded eigenvalues. Furthermore, there is no singular continuous spectrum, cf. [6]. 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 [15,16] 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 [5,1]: 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 ∞. 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

$$W_t(x,y) := \begin{cases} V(x,y), & x \geqslant 0, \\ V(x+t,y), & x < 0, \end{cases} \tag{1.2}$$

for $t \in [0,1]$. On the strip Σ 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 [6,10]), 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 $J \subset \mathbb{R} \backslash \sigma(D_0)$ are open intervals and $\overline{J} \subset \mathbb{R} \backslash \sigma(D_0)$. 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 [13].

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 [7] 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 Σ. 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 Appendix A 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 [14,19].

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 $C_c^\infty(\mathbb{R})$. Our basic class of potentials is given by

$$\mathcal{P} := \{ V \in L_{1,\text{loc}}(\mathbb{R}, \mathbb{R}); \forall x \in \mathbb{R}: \ V(x+1) = V(x) \}. \tag{2.1}$$

Potentials $V \in \mathcal{P}$ belong to the class $L_{1,\text{loc,unif}}(\mathbb{R})$ which coincides with the Kato-class on the real line; in particular, any $V \in \mathcal{P}$ 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. [3]). For $V \in \mathcal{P}$ given, we define the dislocation potentials W_t as in Eq. (1.1), for $0 \leqslant t \leqslant 1$; 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 [8,20], we have

$$\sigma(H) = \sigma_{\text{ess}}(H) = \bigcup_{k=1}^{\infty} [\gamma_k, \gamma_k'], \tag{2.2}$$

where the γ_k and γ_k' satisfy $\gamma_k < \gamma_k' \leqslant \gamma_{k+1}$, 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

$$H_D = H^- \oplus H^+, \qquad H_{t,D} = H_t^- \oplus H_{(-t,0)} \oplus H^+, \tag{2.3}$$

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. The eigenvalues of H_t in the gaps of H depend continuously on t; cf. Appendix A 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 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 2.1. *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 $f_j : (\alpha_j, \beta_j) \to \Gamma_k$, where $0 \leqslant \alpha_j < \beta_j \leqslant 1$, 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 Appendix A. Under stronger assumptions on V one can show that the eigenvalue branches are Hölder- or Lipschitz-continuous, or even analytic; cf. Appendix A. Additional information on the eigenvalue functions f_j can be found in [15,16].

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 $f_i(\alpha_i) := \lim_{t\downarrow\alpha_i} f_i(t)$, $f_i(\beta_i) := \lim_{t\uparrow\beta_i} f_i(t)$, we now define

$$\mathcal{N}_k := \#\{i \mid f_i(\alpha_i) = \gamma_{k+1},\ f_i(\beta_i) = \gamma_k'\} - \#\{i \mid f_i(\alpha_i) = \gamma_k',\ f_i(\beta_i) = \gamma_{k+1}\}. \tag{2.4}$$

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 2.2. *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 [15,16] 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. For further reading concerning the spectral flow through the gaps of perturbed Schrödinger operators, we recommend [18,22].

The main idea of our proof—somewhat reminiscent of [5,1]—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. [8,20]) 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 2.2 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 2.3. *The eigenvalues of $H_{n,t}$ depend continuously on $t \in [0, 1]$.*

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

$$U_{n,t} : L_2(-n-t,n) \to L_2(-n,n), \qquad (U_{n,t}f)(x) := \sqrt{\sigma_{n,t}}\, f(\sigma_{n,t}x), \tag{2.5}$$

where $\sigma_{n,t} := \frac{2n+t}{2n}$. Let $\widetilde{H}_{n,t} := U_{n,t}H_{n,t}U_{n,t}^{-1}$ and $\widetilde{W}_t(x) := W_t(\sigma_{n,t}x)$ so that (writing $\sigma = \sigma_{n,t}$)

$$\widetilde{H}_{n,t} = \sigma^{-2}h_0 + \widetilde{W}_t(x) = \sigma^{-2}\big(h_0 + \sigma^2\widetilde{W}_t(x)\big). \tag{2.6}$$

It is easy to see that the mapping $[0,1] \ni t \mapsto \sigma^2\widetilde{W}_t \in L_1(-n,n)$ is continuous. Now the usual perturbational and variational arguments for quadratic forms ([14] and Appendix A) imply that the eigenvalues of $h_0 + \sigma^2\widetilde{W}_t$ 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 $0 \leqslant t \leqslant 1$ 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 $0 \leqslant \varphi \leqslant 1$ and $\varphi(x) = 1$ for $|x| \leqslant 1$. For $k \in (0,\infty)$ we then define $\varphi_k(x) := \varphi(x/k)$ so that $\operatorname{supp}\varphi_k \subset (-2k,2k)$, $\varphi_k(x) = 1$ for $|x| \leqslant k$, $|\varphi_k'(x)| \leqslant Ck^{-1}$ and $|\varphi_k''(x)| \leqslant Ck^{-2}$. 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 $n \geqslant n_0$, and*

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

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

$$\|H_{n,t}u_k - Eu_k\| \leqslant 2 \cdot \|\varphi_k'\|_\infty \|u'\| + \|\varphi_k''\|_\infty \|u\|, \tag{2.8}$$

it is now easy to conclude that $\dim P_{(\eta_1,\eta_2)}(H_{n,t}) \geqslant \dim P_{(\eta_1,\eta_2)}(H_t)$ 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 $(n_j)_{j\in\mathbb{N}} \subset \mathbb{N}$ such that $\eta \in \sigma(H_{n_j,t})$; we let $u_{n_j,t} \in D(H_{n_j,t})$ denote a normalized eigenfunction and set

$$v_{1,n_j} := \varphi_{k_j}u_{n_j,t}, \qquad v_{2,n_j} := \psi_{k_j}u_{n_j,t}, \tag{2.9}$$

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 $\|u_{n,t}'\|$ 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

$$\tilde{v}_{2,n_j} := \begin{cases} v_{2,n_j}(x), & x \geqslant 0, \\ v_{2,n_j}(x-t), & x < 0, \end{cases} \tag{2.10}$$

belongs to the domain of $H_{n_j,0}$ and $H_{n_j,0}\tilde{v}_{2,n_j} = [H_{n_j,t}v_{2,n_j}]^\sim$, where $[\cdot]^\sim$ is defined in analogy with Eq. (2.10). Since we also have $(H_{n_j,t} - \eta)v_{2,n_j} \to 0$, as $j \to \infty$, we see that $(H_{n_j,0} - \eta)\tilde{v}_{2,n_j} \to 0$. But $\operatorname{dist}(\eta, \sigma(H_{n,0})) \geqslant \delta_0 > 0$ for all n and the Spectral Theorem implies that $\|\tilde{v}_{2,n_j}\| \to 0$ 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 $\dim P_{(\eta_1,\eta_2)}(H_{n,t}) \leqslant \dim P_{(\eta_1,\eta_2)}(H_t)$, 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 2.5. In fact, using standard exponential decay estimates for resolvents of Schrödinger operators, cf. [21], 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 $c \geqslant 0$ and $\alpha > 0$ such that the operators $H_{n,t}$ have an eigenvalue in $(E - c\mathrm{e}^{-\alpha n}, E + c\mathrm{e}^{-\alpha n})$, 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 $(H_{n,t})_{0\leqslant t\leqslant 1}$ and $(H_t)_{0\leqslant t\leqslant 1}$ 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 $0 = t_0 < t_1 < \cdots < t_{K-1} < t_K = 1$ and there exist $E_j \in \Gamma_k$ and $n_0 \in \mathbb{N}$ such that*

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

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 $\eta_t \notin \sigma(H_\tau)$ for all $\tau \in (t-\varepsilon_t, t+\varepsilon_t)$. By compactness, we can find a partition $(\tau_j)_{0 \leqslant j \leqslant K}$ (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 $j = 1, \dots, K-1$, set $t_0 = 0$, $t_K = 1$ and see that $E_j \notin \sigma(H_t)$ for $t_{j-1} \leqslant t \leqslant t_j$, $j = 1, \dots, K$. 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 $\mathcal{N}_k$ as in Eq. (2.4). We fix some $\widetilde{E} \in \Gamma_k$ such that $\widetilde{E} > E_j$ for $j = 0, \dots, K$ and $\widetilde{E} \notin \sigma(H_{t_j}) \cup \sigma(H_{n,t_j})$ for $j = 0, \dots, K$ and for all n large. It is then easy to see that

$$\mathcal{N}_k = \sum_{j=1}^{K} \big(\dim P_{(E_j, \widetilde{E})}(H_{t_j}) - \dim P_{(E_j, \widetilde{E})}(H_{t_{j-1}}) \big) \tag{2.12}$$

and that

$$\dim P_{(-\infty, \widetilde{E})}(H_{n,1}) - \dim P_{(-\infty, \widetilde{E})}(H_{n,0}) = \sum_{j=1}^{K} \big(\dim P_{(E_j, \widetilde{E})}(H_{n,t_j}) - \dim P_{(E_j, \widetilde{E})}(H_{n,t_{j-1}}) \big). \tag{2.13}$$

The left-hand side of (2.13) equation equals k. Furthermore, by Lemma 2.4, we have

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

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 2π-periodic potential

$$V(x) := \begin{cases} -1, & x \in [0, \pi], \\ 1, & x \in (\pi, 2\pi). \end{cases} \tag{3.1}$$

(While the other sections of this paper 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 $H = -\frac{d^2}{dx^2} + V$, we compute the discriminant function

$$D(E) := \varphi_1(2\pi; E) + \varphi_2'(2\pi; E) = \operatorname{tr} \begin{pmatrix} \varphi_1(2\pi; E) & \varphi_1'(2\pi; E) \\ \varphi_2(2\pi; E) & \varphi_2'(2\pi; E) \end{pmatrix} \tag{3.2}$$

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

$$-u'' + (V - E)u = 0 \tag{3.3}$$

and satisfy the boundary conditions

$$\varphi_1(0; E) = \varphi_2'(0; E) = 1 \quad \text{and} \quad \varphi_1'(0; E) = \varphi_2(0; E) = 0. \tag{3.4}$$

The matrix $M(E)$ on the right-hand side of (3.2) 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 $-\frac{d^2}{dx^2} + V$ in $L_2(0, 2\pi)$, cf., e.g., [8,4].

As explained in [8,20], 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 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.,

$$\varphi_-(t; E) = \varphi_+(0; E) \quad \text{and} \quad \varphi_-'(t; E) = \varphi_+'(0; E). \tag{3.5}$$

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. [7]. 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

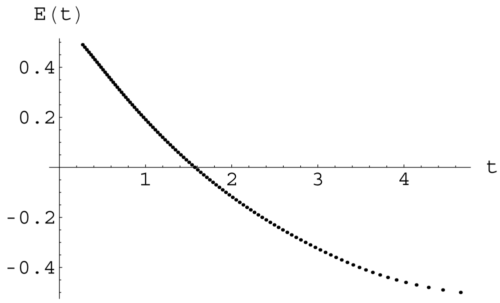

Fig. 1. An eigenvalue branch of H_t in the first spectral gap.

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

$$\left|\frac{\varphi_-(t;E)}{\varphi'_-(t;E)} - \frac{\varphi_+(0;E)}{\varphi'_+(0;E)}\right| < \varepsilon, \tag{3.6}$$

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 Eq. (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., $\sigma_{\mathrm{ess}}(S_t) = \sigma_{\mathrm{ess}}(S_0)$ 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 Σ. Let

$$\Sigma_{n,t} := (-n - t, n) \times (0,1), \quad n \in \mathbb{N}, \tag{4.1}$$

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., [20,8]), 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 $\|\nabla u_n\| \leqslant C$ for some constant $C \geqslant 0$. We now choose cut-off functions φ_n as in Section 2 and denote the natural extension to $\mathbb{R}^2$ again by φ_n. We also let $\psi_n = 1 - \varphi_n$. Clearly,

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

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

$$\big\|(S_{\bar{t}} - E)(\varphi_{n_j/4} u_{n_j})\big\| \to 0, \quad j \to \infty, \tag{4.3}$$

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 $\tilde{v} : \Sigma_{n,0} \to \mathbb{C}$ by

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

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

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

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 $[\psi_{n/4}u_n]^\sim \to 0$ (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 $\|(S_{\hat t}-E)v_{n_j}\|\to 0$ and $\|v_{n_j}\|\to 1$ as $j\to\infty$ which implies $E\in\sigma(S_{\hat t})$. □

Remark 4.2. By a well-known line of argument, one can obtain *exponential localization* of the eigenfunctions of S_t near the interface $\{(x,y)\mid x=0\}$. Since we will use exponential localization in a more systematic way in the forthcoming paper [13] we only give a brief sketch here: 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 4.1. As above, we have

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

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

$$\|\chi_{|x|\geqslant 4n}u\| \leqslant \big\|\chi_{|x|\geqslant 4n}(S_t-E)^{-1}r_n\big\| \leqslant C\mathrm{e}^{-\alpha n}, \tag{4.7}$$

by standard exponential decay estimates for the resolvent kernel of Schrödinger operators (cf., e.g., [21,13]).

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

$$D_t = -\Delta + W_t, \quad 0\leqslant t\leqslant 1. \tag{4.8}$$

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

$$D_t \simeq \int_{[0,2\pi]}^{\oplus} S_t(\vartheta)\frac{\mathrm{d}\vartheta}{2\pi}, \tag{4.9}$$

and hence the spectrum of D_t has a band-gap structure; furthermore, D_t has no singular continuous part, cf. [6,11]. 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, $a>\inf\sigma_{\mathrm{ess}}(D_0)$, 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 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

$$\begin{aligned}(D_t-E)(\Phi_n\tilde u_n) &= \big(-\partial_x^2-\partial_y^2+W_t-E\big)\big(\varphi_n(x)\varphi_n(y)\tilde u_n(x,y)\big)\\ &= \varphi_n(y)\big[(S_t-E)\big(\varphi_n(x)u_n\big)\big]^\sim - \varphi_n(x)\big(2\varphi_n'(y)\partial_y\tilde u_n + \varphi_n''(y)\tilde u_n\big).\end{aligned} \tag{4.10}$$

The norms of the three terms on the right-hand side 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

$$\big\|(D_t-E)(\Phi_n\tilde u_n)\big\| \leqslant c_0(1+n\varepsilon), \tag{4.11}$$

while $\|\Phi_n\tilde u_n\|\geqslant c_0 n$ with a constant $c_0>0$. This implies the desired result. □

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

$$v_n = v_n(x,y) := \frac{1}{\|\Phi_n\tilde u_n\|}\Phi_n\tilde u_n \tag{4.12}$$

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

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

These functions play a key role in our analysis of the rotation problem at small angle in [13].

We finally turn to a brief discussion of the i.d.s. (the integrated density of states [24]) for the dislocation operators D_t. We adopt the natural distinction of [6,10,17] 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 $\overline{J} \subset \mathbb{R} \setminus \sigma(D_0)$

$$\rho_{\text{bulk}}(I, D_t) = \lim_{n\to\infty} \frac{1}{4n^2} N\big(I, D_t^{(n)}\big), \qquad \rho_{\text{surf}}(J, D_t) = \lim_{n\to\infty} \frac{1}{2n} N\big(J, D_t^{(n)}\big). \tag{4.14}$$

The existence of the limits in (4.14) has been established in [10,17] 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 Eq. (4.14) is not suited to capture the surface states (cf. [10,17]).

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 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 $\|u_0\| = 1$, $\operatorname{supp} u_0$ compact, and $\|(D_t - E)u_0\| < \varepsilon$. Let $\nu \in \mathbb{N}$ be such that $\operatorname{supp} u_0 \subset (-\nu, \nu)^2$; note that, in the present proof, ν corresponds to the n of Remark 4.4. 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 $\operatorname{supp} \varphi_k \subset (-n, n)^2$ provided $(2k + 1)\nu < n$. Denoting $\mathcal{M}_n := \operatorname{span}\{\varphi_k \mid k \in \mathbb{N},\ k \leqslant \frac{1}{2}(\frac{n}{\nu} - 1)\}$, it is clear that $\dim \mathcal{M}_n \geqslant n/(3\nu)$, 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 $\dim \mathcal{N}_n \geqslant \dim \mathcal{M}_n$ 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, $\|(D_t^{(n)} - E)v\| \geqslant \varepsilon$. On the other hand, v is a finite linear combination of the φ_k, which implies $\|(D_t^{(n)} - E)v\| < \varepsilon$. □

We will continue the discussion of bulk versus surface states in the companion paper [13] where a corresponding upper bound of the form $N(J, D_t^{(n)}) \leqslant cn \log n$ 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

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

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 $\bigoplus_{(i,j)\in\mathbb{Z}^2} H_{ij}$. Without loss of generality, we may assume $y_0 = 0$ henceforth.

5.1. 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 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

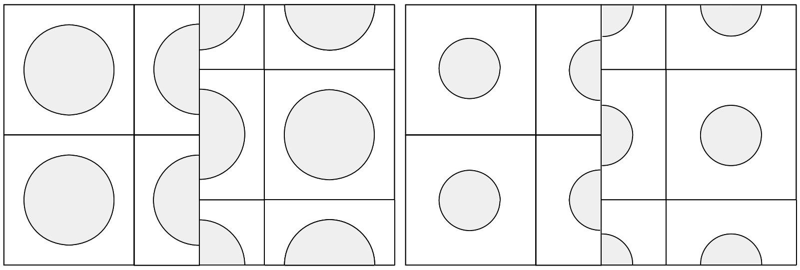

Fig. 2. Muffin tins: two cases for dislocation in the y-direction.

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 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 [13] 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 $n \to \infty$.

5.2. 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 $\widetilde{W}_t$ coincide with V in the right half-plane, while we take $\widetilde{W}_t(x, y) = V(x, y - t)$ 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. Fig. 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 $0 \leqslant t \leqslant \tau_0$ and for $\tau_1 \leqslant t \leqslant 1$; 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 [23]; cf. also [6]. 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.

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Appendix A. 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 $\mathcal{P} \subset L_{1,\mathrm{loc},\mathrm{unif}}(\mathbb{R})$ as in (2.1) where the eigenvalues are continuous functions of the dislocation parameter t. In the subsequent estimates we will use

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

as a natural norm on $L_{1,\mathrm{loc},\mathrm{unif}}(\mathbb{R})$. As is well known (cf., e.g., [3]), any potential $V \in L_{1,\mathrm{loc},\mathrm{unif}}(\mathbb{R})$ is relatively form-bounded with respect to h_0 with relative form-bound zero. More precisely, we have the following lemma.

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

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

Proof. For $f \in C_c^\infty(\mathbb{R})$ with support contained in $(0,\varepsilon)$ we have $\|f\|_\infty \leqslant \sqrt{\varepsilon}\|f'\|$. 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 (see [3]), we have for any $\varphi \in C_c^\infty(\mathbb{R})$,

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

so that

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

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

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

$$\vartheta_V(s) := \int_0^1 |V(x+s) - V(x)|\,\mathrm{d}x, \quad 0 \leqslant s \leqslant 1, \tag{A.3}$$

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

Lemma A.2. *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 $C \geqslant 0$ such that for some $\tau_1 \in (0, \tau_0)$*

$$\|(H_t - E_0)^{-1} - (H_{t_0} - E_0)^{-1}\| \leqslant C\vartheta_V(t - t_0), \quad |t - t_0| < \tau_1. \tag{A.4}$$

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

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

with some constant C_1. The desired result now follows by [14, 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. We are now prepared for the proof of Lemma 2.1.

Proof of Lemma 2.1. 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 $\sigma(H_t) \cap (\eta_1,\eta_2) = \emptyset$, or
Type (2): η is an eigenvalue of H_τ 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 (η_1,η_2), for $\tau_1 < t < \tau_2$.

Now the family $\{U_{\eta,\tau} \mid (\eta,\tau) \in (a,b) \times \mathbb{T}\}$ 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

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

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 $f : (\tau_1,\tau_2) \to (\eta_1,\eta_2)$ 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 $\tilde{f}:(\alpha,\beta) \to (a,b)$ 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 2.1. With $\vartheta_V:[0,1] \to [0,\infty)$ as in (A.3), we study potentials from the classes

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

where $0 < \alpha \leqslant 1$. 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. 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 $V \in \mathcal{P}_1$.

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

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

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

$$\|(H_t - E_j)^{-1} - (H_{t'} - E_j)^{-1}\| \leqslant c_j|t-t'|, \quad t,t' \in I_j.$$

This implies that the min–max-values $\mu_k(s)$ of $(H_s - E_j)^{-1}$ satisfy

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

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 $C := \max\{c_1,\dots,c_\ell\}$ to finish our proof. □

Remarks A.4. (a) By the same argument, we obtain the following result on Hölder-continuity: If $0 < \alpha < 1$ and $V \in \mathcal{P}_\alpha$, then each of the functions $f_j:(\alpha_j,\beta_j) \to (a,b)$ is locally uniformly Hölder-continuous (as defined in [12]), 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 $|f_j(t) - f_j(t')| \leqslant C|t-t'|^\alpha$, 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.

(b) For analytic potentials V, it is shown in [15] 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 [16], the author proves that the f_j are squares of W_2^1-functions near the gap edges if the potential is in $L_2(\mathbb{T})$.

We finally give a characterization of the class $\mathcal{P}_1$.

Proposition A.5. *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 result due to J. Voigt, Dresden; cf. also [9, Chapter 5] for related material on BV-functions of several variables.

Lemma A.6. *Let $f \in L_{1,\mathrm{loc}}(\mathbb{R}, \mathbb{R})$ be periodic with period 1 and suppose that there are $c \geqslant 0$, $\varepsilon > 0$ such that*

$$\int_0^1 \left| f(x+t) - f(x) \right| \mathrm{d}x \leqslant ct, \quad \forall 0 < t < \varepsilon. \tag{A.6}$$

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

We then have: the distributional derivative ∂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 $\eta : C^1(\mathbb{T}) \to \mathbb{R}$ by

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

we may compute

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

and the assumption (A.6) yields the estimate $|\eta(\varphi)| \leqslant c\|\varphi\|_\infty$. 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

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

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

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